

NBO 2018 – 1969 references  
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Ababsa, S.; Zouchoune, B.

ELECTRONIC STRUCTURE AND RELATIVE STABILITIES OF 10-AND 12-VERTEX. CLOSO- AND NIDO-HETEROBORANE CLUSTERS OF Ga, Ge, AND As ELEMENTS

Journal of Structural Chemistry, (59): 276-289. 2018. 10.1134/s002247661802004x

Abbasi, A.; Sardroodi, J. J.

A highly sensitive chemical gas detecting device based on N-doped ZnO as a modified nanostructure media: A DFT plus NBO analysis

Surface Science, (668): 150-163. 2018. 10.1016/j.susc.2017.10.029

Abbasi, A.; Sardroodi, J. J.

Investigation of the adsorption of ozone molecules on TiO<sub>2</sub>/WSe<sub>2</sub> nanocomposites by DFT computations: Applications to gas sensor devices

Applied Surface Science, (436): 27-41. 2018. 10.1016/apsusc.2017.12.010

Abbenseth, J.; Bete, S. C.; Finger, M.; Volkmann, C.; Wurtele, C.; Schneider, S.

Four- and Five-Coordinate Osmium(IV) Nitrides and Imides: Circumventing the "Nitrido Wall"  
Organometallics, (37): 802-811. 2018. 10.1021/acs.organomet.7b00707

Abdel-Latif, S. A.; Mohamed, A. A.

Novel Zn(II) complexes of 1,3-diphenyl-4-(arylazo)pyrazol-5-one derivatives: Synthesis, spectroscopic properties, DFT calculations and first order nonlinear optical properties

Journal of Molecular Structure, (1156): 712-725. 2018. 10.1016/j.molstruc.2017.12.028

Abdel-Latif, S. A.; Mohamed, A. A.

Synthesis, spectroscopic characterization, first order nonlinear optical properties and DFT calculations of novel Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) complexes with 1,3-diphenyl-4-phenylazo-5-pyrazolone ligand

Journal of Molecular Structure, (1153): 248-261. 2018. 10.1016/j.molstruc.2017.10.002

Abdel-Latif, S. A.; Moustafa, H.

Synthesis, spectroscopic properties, density functional theory calculations and nonlinear optical properties of novel complexes of 5-hydroxy-4,7-dimethyl-6-(phenylazo)coumarin with Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) metal ions

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4269

Abdelmoula, H.; Trabelsi, S.; Nasr, S.; Bellissent-Funel, M. C.

Hydrogen-bond network in liquid Formamide Methanol mixture as studied by neutron scattering and density functional theory

Journal of Molecular Liquids, (271): 8-15. 2018. 10.1016/j.molliq.2018.08.131

Abdel-Rahman, L. H.; Adam, M. S. S.; Abu-Dief, A. M.; Moustafa, H.; Basha, M. T.; Aboraia, A. S.; Al-Farhan, B. S.; Ahmed, H. E.

Synthesis, theoretical investigations, biocidal screening, DNA binding, in vitro cytotoxicity and molecular docking of novel Cu (II), Pd (II) and Ag (I) complexes of chlorobenzylidene Schiff base: Promising antibiotic and anticancer agents

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4527

Abdolmaleki, A.; Dadsetani, M.; Zabardasti, A.

Improving the first hyperpolarizability of anthracene through interaction with HX molecules (X=F, Cl, Br): A theoretical study

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (196): 353-365. 2018. 10.1016/j.saa.2018.02.042

Abdulsattar, M. A.; Abduljalil, H. M.; Khaleel, M. K.

Structural and Spectroscopic Properties of AlAs Diamondoids: An Approach to Nanocrystals and Bulk Properties

Chiang Mai Journal of Science, (45): 547-555. 2018.

Abedini, F.; Omidyan, R.

Excited-State Proton Transfer in Thiazolo- 4, 5-d thiazo Heterocyclic Systems and the Geometry Alterations' Effect on Photophysical Characters: A Theoretical Study

Journal of Physical Chemistry A, (122): 2653-2662. 2018. 10.1021/acs.jpca.7b09593

Abiram, A.; Praveena, G.

Exploring the structure and stability of beta-dipeptide - A quantum chemical and molecular dynamics study

Indian Journal of Pure & Applied Physics, (56): 561-569. 2018.

Abraham, C. S.; Muthu, S.; Prasana, J. C.; Rizwana, B. F.; Armakovic, S.; Armakovic, S. J.

Vibrational and electronic absorption spectroscopic profiling, natural hybrid orbital, charge transfer, electron localization function and molecular docking analysis on 3-amino-3-(2-nitrophenyl) propionic acid

Journal of Molecular Structure, (1171): 733-746. 2018. 10.1016/j.molstruc.2018.06.057

Abraham, C. S.; Prasana, J. C.; Muthu, S.; Rizwana, B. F.; Raja, M.

Quantum computational studies, spectroscopic (FT-IR, FT-Raman and UV-Vis) profiling, natural hybrid orbital and molecular docking analysis on 2,4 Dibromoaniline

Journal of Molecular Structure, (1160): 393-405. 2018. 10.1016/j.molstruc.2018.02.022

Abtouche, S.; Issad-Elkebich, M.; Brahimi, M.; Assfeld, X.

Complexation of Ca<sup>2+</sup> cation by the lateral chain of Paclitaxel (N-Benzoyl-(ss)-phenylisoserine): A theoretical study

Computational and Theoretical Chemistry, (1146): 1-9. 2018. 10.1016/j.comptc.2018.11.001

Achour, S.; Seydou, M.; Maurel, F.; Tangour, B.

Intramolecular hydrogenation of triethylsilylethylene catalyzed by Ru(II) complex: Agostic bond formation and trizonal transition states with ten acting atoms

Inorganica Chimica Acta, (469): 536-544. 2018. 10.1016/j.ica.2017.10.013

Acosta-Silva, C.; Bertran, J.; Branchadell, V.; Oliva, A.

Phosphoryl-Transfer Reaction in RNA under Alkaline Conditions

Chemistry-a European Journal, (24): 13565-13572. 2018. 10.1002/chem.201802332

Adeniyi, A. A.; Conradie, J.

The stability, kinetics and inter-fragment electron communication of the tautomers of twelve selected beta-diketone molecules: A computational study

Journal of Molecular Graphics & Modelling, (85): 25-39. 2018. 10.1016/j.jmgm.2018.06.019

Adjieufack, A. I.; Liegeois, V.; Mboumbouo, I. N.; Mbadcam, J. K.; Champagne, B.

Intramolecular 3+2 Cycloaddition Reactions of Unsaturated Nitrile Oxides. A Study from the Perspective of Bond Evolution Theory (BET)

Journal of Physical Chemistry A, (122): 7472-7481. 2018. 10.1021/acs.jpca.8b06711

Adonin, S. A.; Udalova, L. I.; Abramov, P. A.; Novikov, A. S.; Yushina, I. V.; Korolkov, I. V.; Semitut, E. Y.; Derzhavskaya, T. A.; Stevenson, K. J.; Troshin, P. A.; Sokolov, M. N.; Fedin, V. P.

A Novel Family of Polyiodo-Bromoantimonate(III) Complexes: Cation-Driven Self-Assembly of Photoconductive Metal-Polyhalide Frameworks

Chemistry-a European Journal, (24): 14707-14711. 2018. 10.1002/chem.201802100

Afshari, T.; Mohsennia, M.

A molecular electron density theory study of the asymmetric hetero-Diels-Alder cycloaddition reaction between ferrocenyl-substituted thiabutadiene and methyl propiolate

Computational and Theoretical Chemistry, (1140): 117-124. 2018.

10.1016/j.comptc.2018.08.005

Afzali, R.; Vakili, M.; Boluri, E.; Tayyari, S. F.; Nekoei, A. R.; Hakimi-Tabar, M.; Darugar, V.

Structure, isomerism, and vibrational assignment of aluminumtrifluoroacetylacetone. An experimental and theoretical study

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (190): 15-22. 2018.

10.1016/j.saa.2017.08.075

Aghaei, S. M.; Monshi, M. M.; Torres, I.; Zeidi, S. M. J.; Calizo, I.

DFT study of adsorption behavior of NO, CO, NO<sub>2</sub>, and NH<sub>3</sub> molecules on graphene-like BC<sub>3</sub>: A search for highly sensitive molecular sensor

Applied Surface Science, (427): 326-333. 2018. 10.1016/j.apsusc.2017.08.048

Agirre, M.; Henrion, S.; Rivilla, I.; Miranda, J. I.; Cossio, F. P.; Carboni, B.; Villalgordo, J. M.; Carreaux, F.

1,3-Dioxa- 3,3 -sigmatropic Oxo-Rearrangement of Substituted Allylic Carbamates: Scope and Mechanistic Studies

Journal of Organic Chemistry, (83): 14861-14881. 2018. 10.1021/acs.joc.8b01320

Agirtas, M. S.; Cabir, B.; Gumus, S.; Ozdemir, S.; Dundar, A.

Synthesis and antioxidant, aggregation, and electronic properties of 6-tert-butyl-1,4-benzodioxine substituted phthalocyanines

Turkish Journal of Chemistry, (42): 100-111. 2018. 10.3906/kim-1605-59

Agou, T.; Ohata, R.; Mizuhata, Y.; Tokitoh, N.; Fukumoto, H.; Kubota, T.

Synthesis of a new highly-fluorinated cis-1,2-cyclopentanediol and its application for fluorinated oligoesters

Journal of Fluorine Chemistry, (210): 78-82. 2018. 10.1016/j.jfluchem.2018.03.002

Aguilar, E. C.; Echeverria, G. A.; Piro, O. E.; Ulic, S. E.; Jios, J. L.; Tuttolomondo, M. E.; Perez, H.

Weak and strong hydrogen bonds conducting the supramolecular framework of 1-butyl-3-(1-naphthoyl)thiourea: crystal structure, vibrational studies, DFT methods, Pixel energies and Hirshfeld surface analysis

Molecular Physics, (116): 399-413. 2018. 10.1080/00268976.2017.1395917

Aguilar-Galindo, F.; Diaz-Tendero, S.

Theoretical Insights into Vinyl Derivatives Adsorption on a Cu(100) Surface

Journal of Physical Chemistry C, (122): 27301-27313. 2018. 10.1021/acs.jpcc.8b06142

Aguilar-Galindo, F.; Ocon, P.; Poyato, J. M. L.

Exploring the catalytic efficiency of X-doped (X=B, N, P) graphene in oxygen reduction reaction: Influence of solvent and border effects

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25579

Ahlburg, N. L.; Doppelb, O.; Hillrichs, K.; Namyslo, J. C.; Hubner, E. G.; Schmidt, A.

DEPROTONATION OF 4-ETHYNYL PYRAZOLIUM SALTS

Heterocycles, (96): 1203-1215. 2018. 10.3987/com-18-13916

Ahmad, M. S.; Khalid, M.; Shaheen, M. A.; Tahir, M. N.; Khan, M. U.; Braga, A. A. C.; Shad, H. A.

Synthesis and XRD, FT-IR vibrational, UV-vis, and nonlinear optical exploration of novel tetra substituted imidazole derivatives: A synergistic experimental-computational analysis

Journal of Physics and Chemistry of Solids, (115): 265-276. 2018. 10.1016/j.jpcs.2017.12.054

Ahmadi, A.; Kassaee, M. Z.; Fattahi, A.

Does gold cluster promote or scavenge radicals? A controversy at DFT

Journal of Physical Organic Chemistry, (31) 2018. 10.1002/poc.3776

Ahmadi, S.; Marino, T.; Prejano, M.; Russo, N.; Toscano, M.

Antioxidant Properties of the Vam3 Derivative of Resveratrol

Molecules, (23) 2018. 10.3390/molecules23102446

Ai, L. Y.; Zhao, H. Y.; Ma, H. M.; Wang, J.; Liu, Y.  
Ti<sub>12</sub>C<sub>68</sub>: A stable T-h-symmetry hollow cage  
Scientific Reports, (8) 2018. 10.1038/s41598-018-22381-y

Aicher, F. S. W.; Eichele, K.; Schubert, H.; Wesemann, L.  
Complete Hydrogen Transfer: Tin Hydride Reactivity toward Adamantylisonitrile and Benzonitrile  
Organometallics, (37): 1773-1780. 2018. 10.1021/acs.organomet.8b00207

Akbar, R.; Baral, M.; Kanungo, B. K.  
Synthesis, thermodynamic, photophysical and DFT studies of some trivalent metal chelates of a hexadentate tripodal hydroxyquinolate-based ligand  
Journal of Coordination Chemistry, (71): 135-154. 2018. 10.1080/00958972.2018.1430362

Aksamentova, T. N.; Chipanina, N. N.; Oznobikhina, L. P.; Adamovich, S. N.; Smirnov, V. I.  
Molecular structure, proton affinity and hydrogen bonds of (2-hydroxyethyl)amine-N-oxides: DFT, MP2 and FTIR study  
Journal of Molecular Structure, (1151): 142-151. 2018. 10.1016/j.molstruc.2017.09.013

Al Furaiji, K. H. M.; Iversen, K. J.; Dutton, J. L.; Wilson, D. J. D.  
Theoretical Investigation of Hydride Insertion into N-Heterocyclic Carbenes Containing N, P, C, O and S Heteroatoms  
Chemistry-an Asian Journal, (13): 3745-3752. 2018. 10.1002/asia.201801285

Alam, M.; Alam, M. J.; Azaz, S.; Parveen, M.; Park, S.; Ahmad, S.  
DFT/TD-DFT calculations, spectroscopic characterizations (FTIR, NMR, UV-vis), molecular docking and enzyme inhibition study of 7-benzoyloxycoumarin  
Computational Biology and Chemistry, (73): 65-78. 2018. 10.1016/j.compbiochem.2018.01.007

Alam, M.; Park, S.  
Molecular structure, spectral studies, NBO, HOMO-LUMO profile, MEP and Mulliken analysis of 3 beta,6 beta,-dichloro-5 alpha-hydroxy-5 alpha-cholestane  
Journal of Molecular Structure, (1159): 33-45. 2018. 10.1016/j.molstruc.2018.01.043

Alamiddine, Z.; Thany, S.; Graton, J.; Le Questel, J. Y.  
Conformations and Binding Properties of Thiametoxam and Clothianidin Neonicotinoid Insecticides to Nicotinic Acetylcholine Receptors: The Contribution of sigma-Hole Interactions  
Chemphyschem, (19): 3069-3083. 2018. 10.1002/cphc.201800656

Al-Amri, A. H.; Elroby, S. A.; Hilal, R. H.  
Theoretical insight into the structure and bonding characteristics of Bisphenol-A. QTAIM and NBO analyses

Al-Ansari, I. A. Z.

Role of Solvent Polarity and Hydrogen-Bonding on Excited-State Fluorescence of 3- (E)-{4-Dimethylamino benzylidene}amino -2-naphthoic Acid (DMAMN): Isomerization vs Rotomerization  
Journal of Physical Chemistry A, (122): 1838-1854. 2018. 10.1021/acs.jpca.7b11623

Al-Azmi, A.; Shalaby, M. A.

Experimental and computational approaches to the analysis of the molecular structure of (E)-3-(3-(4-nitrophenyl)triaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile  
Journal of Molecular Structure, (1155): 239-248. 2018. 10.1016/j.molstruc.2017.11.006

Albertin, G.; Antoniutti, S.; Castro, J.; Ganz, V.; Sibilla, F.

Preparation and reactivity of half-sandwich organic azide complexes of osmium  
Dalton Transactions, (47): 11658-11668. 2018. 10.1039/c8dt02230e

Alcoba, D. R.; Ona, O. B.; Torre, A.; Lain, L.; Tiznado, W.

An orbital localization criterion based on the topological analysis of the electron localization function at correlated level

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25588

Alexander, G. V.; Rosero-Navarro, N. C.; Miura, A.; Tadanaga, K.; Murugan, R.

Electrochemical performance of a garnet solid electrolyte based lithium metal battery with interface modification

Journal of Materials Chemistry A, (6): 21018-21028. 2018. 10.1039/c8ta07652a

Alghanmi, R. M.; Soliman, S. M.; Basha, M. T.; Habeeb, M. M.

Electronic spectral studies and DFT computational analysis of hydrogen bonded charge transfer complexes between chloranilic acid and 2,5-dihydroxy-p-benzoquinone with 2-amino-4-methylbenzothiazole in methanol

Journal of Molecular Liquids, (256): 433-444. 2018. 10.1016/j.molliq.2018.02.056

Ali, N.; Mansha, A.; Asim, S.; Zahoor, A. F.; Ghafoor, S.; Akbar, M. U.

A computational perspective of vibrational and electronic analysis of potential photosensitizer 2-chlorothioxanthone

Journal of Molecular Structure, (1156): 571-582. 2018. 10.1016/j.molstruc.2017.12.015

Ali, R.; Fatemeh, Z. N.; Younes, H.; Sang Woo, J.; Masoome, S.; Katarzyna, S.; Tadeusz, L.; Farideh, G.

Synthesis, Crystal Structure and Theoretical Calculations of N-Benzyl-1-(5-(3-chlorophenyl)-1,3,4-oxadiazol-2-yl)cyclopentanamine

Chinese Journal of Structural Chemistry, (37): 679-+. 2018. 10.14102/j.cnki.0254-5861.2011-1720

Ali, S. M.

Role of Ligand Straining in Complexation of Eu<sup>3+</sup>-Am<sup>3+</sup> Ions by TPEN and PPDEN, Scalar Relativistic DFT Exploration in Conjunction with COSMO-RS  
ACS Omega, (3): 13104-13116. 2018. 10.1021/acsomega.8b00933

Alkorta, I.; Elguero, J.; Del Bene, J. E.  
Complexes of O=C=S with Nitrogen Bases: Chalcogen Bonds, Tetrel Bonds, and Other Secondary Interactions  
Chemphyschem, (19): 1886-1894. 2018. 10.1002/cphc.201800217

Alkorta, I.; Martin-Fernandez, C.; Montero-Campillo, M. M.; Elguero, J.  
Hydrogen-Bonding Acceptor Character of Be-3, the Beryllium Three-Membered Ring  
Journal of Physical Chemistry A, (122): 1472-1478. 2018. 10.1021/acs.jpca.7b11952

Alkorta, I.; Montero-Campillo, M. M.; Elguero, J.; Yanez, M.; Mo, O.  
Trapping One Electron between Three Beryllium Atoms: Very Strong One-Electron Three-Center Bonds  
Chemphyschem, (19): 1068-1074. 2018. 10.1002/cphc.201701240

Allan, N. L.; Dale, H. J. A.; Hart, J. N.; Claeysens, F.  
Adventures in boron chemistry - the prediction of novel ultra-flexible boron oxide frameworks  
Faraday Discussions, (211): 569-591. 2018. 10.1039/c8fd00052b

Almutairi, M. S.; Soumya, S.; Al-Wabli, R. I.; Joe, I. H.; Attia, M. I.  
Density functional theory calculations, vibration spectral analysis and molecular docking of the antimicrobial agent 6-(1,3-benzodioxol-5-ylmethyl)-5-ethyl-2-{ 2-(morpholin-4-yl)ethyl sulfanyl}pyrimidin-4(3H)-one  
Open Chemistry, (16): 653-666. 2018. 10.1515/chem-2018-0067

Almutairi, M. S.; Zakaria, A. S.; Ignasius, P. P.; Al-Wabli, R. I.; Joe, I. H.; Attia, M. I.  
Synthesis, spectroscopic investigations, DFT studies, molecular docking and antimicrobial potential of certain new indole-isatin molecular hybrids: Experimental and theoretical approaches  
Journal of Molecular Structure, (1153): 333-345. 2018. 10.1016/j.molstruc.2017.10.025

Alodia, N.; Jaganade, T.; Priyakumar, U. D.  
Quantum mechanical investigation of the nature of nucleobase-urea stacking interaction, a crucial driving force in RNA unfolding in aqueous urea  
Journal of Chemical Sciences, (130) 2018. 10.1007/s12039-018-1563-8

Al-Otaibi, J. S.; El Gogary, T. M.; El-Demerdash, S. H.  
Umbrella inversion and structure of phosphorus-containing compounds: A quantum chemical study  
Journal of Theoretical & Computational Chemistry, (17) 2018. 10.1142/s0219633618500426

Al-Tamimi, A. M. S.; Mary, Y. S.; Hassan, H. M.; Resmi, K. S.; El-Emam, A. A.; Narayana, B.; Sarojini, B. K.

Study on the structure, vibrational analysis and molecular docking of fluorophenyl derivatives using FT-IR and density functional theory computations

Journal of Molecular Structure, (1164): 172-179. 2018. 10.1016/j.molstruc.2018.03.070

Al-Tamimi, A. M. S.; Mary, Y. S.; Miniyar, P. B.; Al-Wahaibi, L. H.; El-Emam, A. A.; Armakovic, S.; Armakovic, S. J.

Synthesis, spectroscopic analyses, chemical reactivity and molecular docking study and anti-tubercular activity of pyrazine and condensed oxadiazole derivatives

Journal of Molecular Structure, (1164): 459-469. 2018. 10.1016/j.molstruc.2018.03.085

Altarawneh, S. S.; Ababneh, T. S.; Al-Momani, L. A.; Aljaafreh, I. Y.

New Microporous Thiophene-Pyridine Functionalized Imine-Linked Polymer for Carbon-Dioxide Capture

Polymer Science Series B, (60): 789-797. 2018. 10.1134/s1560090419010019

Alturk, S.; Avci, D.; Basoglu, A.; Tamer, O.; Atalay, Y.; Dege, N.

Copper(II) complex with 6-methylpyridine-2-carboxyclic acid: Experimental and computational study on the XRD, FT-IR and UV-Vis spectra, refractive index, band gap and NLO parameters

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (190): 220-230. 2018. 10.1016/j.saa.2017.09.041

Alturk, S.; Avci, D.; Tamer, O.; Atalay, Y.

1H-pyrazole-3-carboxylic acid: Experimental and computational study

Journal of Molecular Structure, (1164): 28-36. 2018. 10.1016/j.molstruc.2018.03.032

Alvarez-Pazos, N.; Albertin, G.; Antoniutti, S.; Bravo, J.; Garcia-Fontan, S.; Hermida-Ramon, J. M.; Zanardo, G.

Trichlorostannyl complexes of Ruthenium(II): Synthesis, structure, reactivity and computational studies

Journal of Organometallic Chemistry, (874): 74-82. 2018. 10.1016/j.jorganchem.2018.08.017

Alvarez-Thon, L.; Mammino, L.

Information on Gas-Phase Diatomic Molecules from Magnetically Induced Current Densities

Journal of Computational Chemistry, (39): 52-60. 2018. 10.1002/jcc.25083

Alver, O.; Parlak, C.; Ramasami, P.; Senyel, M.

Interaction between doped C-60 fullerenes and piperazine-2,3,5,6-tetraone: DFT simulation

Main Group Metal Chemistry, (41): 63-66. 2018. 10.1515/mgmc-2017-0054

Alver, O.; Parlak, C.; Senyel, M.; Ramasami, P.

Density functional theory study on the adsorption of valproic acid to doped fullerenes

Main Group Metal Chemistry, (41): 67-71. 2018. 10.1515/mgmc-2018-0002

Alviri, B. V.; Pourayoubi, M.; Farhadipour, A.; Necas, M.; Bertolasi, V.

A combined X-ray crystallography and theoretical study of N-H center dot center dot center dot OX (X is =P and -C) hydrogen bonds in two new structures with a (C-O)(2)(N)-P(=Y) (Y is O and S) skeleton  
Acta Crystallographica Section C-Structural Chemistry, (74): 1610-+. 2018.  
10.1107/s2053229618014006

Al-Wabli, R. I.; Al-Ghamdi, A. R.; Primsa, I. P.; Ghabbour, H. A.; Al-Agamy, M. H.; Joe, I. H.; Attia, M. I.  
(2E)-2- 1-(1,3-Benzodioxol-5-yl)-3-(1H-imidazol-1-yl)propylidene -N-(4-methoxyphenyl)hydrazinecarboxamide: Synthesis, crystal structure, vibrational analysis, DFT computations, molecular docking and antifungal activity  
Journal of Molecular Structure, (1166): 121-130. 2018. 10.1016/j.molstruc.2018.04.017

Al-Wabli, R. I.; Govindarajan, M.; Almutairi, M. S.; Attia, M. I.  
Spectral characterization, computed frequencies analysis and electronic structure calculations on (1E)-N-hydroxy-3-(1H-imidazol-1-yl)-1-phenylpropan-1-imine: An oxime-bearing precursor to potential antifungal agents  
Journal of Molecular Structure, (1168): 264-279. 2018. 10.1016/j.molstruc.2018.05.022

Al-Wabli, R. I.; Salman, A.; Shyni, V.; Ghabbour, H. A.; Joe, I. H.; Almutairi, M. S.; Maklad, Y. A.; Attia, M. I.  
Synthesis, crystal structure, vibrational profiling, DFT studies and molecular docking of N-(4-chloro-24 2-(1H-indol-2-ylcarbonyl)hydrazinyl (oxo)acetyl)phenyl)acetamide.DMSO: A new antiproliferative agent  
Journal of Molecular Structure, (1155): 457-468. 2018. 10.1016/j.molstruc.2017.10.116

Al-Wahaibi, L. H.; Govindarajan, M.; El-Emam, A. A.; Attia, M. I.  
Spectroscopic (FT-IR, FT-Raman, UV, H-1 and C-13 NMR) insights, electronic profiling and DFT computations on {(E)- 3-(1H-imidazol-1-yl)-1-phenylpropylidene amino}oxy)(4-nitrophenyl)methanone, an imidazole-bearing anti-Candida agent  
Open Chemistry, (16): 50-63. 2018. 10.1515/chem-2018-0005

Amaudrut, J.; Braccini, I.; Duhamel, E.; Montalbetti, C.  
Existence of a Preferred Orientation for the Methoxy Group on an Extended Aromatic System  
Chemistryselect, (3): 6750-6755. 2018. 10.1002/slct.201800881

Amendola, V.; Boiocchi, M.; Fabbrizzi, L.; La Cognata, S.; Legnani, L.; Lo Presti, E.; Mangano, C.; Miljkovic, A.  
Anion-induced isomerization of fluorescent semi(thio)carbazones  
Organic Chemistry Frontiers, (5): 391-397. 2018. 10.1039/c7qo00805h

Amic, A.; Markovic, Z.; Klein, E.; Markovic, J. M. D.; Milenkovic, D.  
Theoretical study of the thermodynamics of the mechanisms underlying antiradical activity of cinnamic acid derivatives  
Food Chemistry, (246): 481-489. 2018. 10.1016/j.foodchem.2017.11.100

An, K.; Zhu, J.

Predicting an unconventional facile route to metallaanthracenes  
Dalton Transactions, (47): 5575-5581. 2018. 10.1039/c8dt00455b

An, M. C.; Du, L.; Du, C. Y.; Sun, Y. R.; Wang, Y. J.; Yin, G. P.; Gao, Y. Z.  
Pt nanoparticles supported by sulfur and phosphorus co-doped graphene as highly active catalyst for acidic methanol electrooxidation  
Electrochimica Acta, (285): 202-213. 2018. 10.1016/j.electacta.2018.07.237

An, P.; Anumula, R.; Wu, H. M.; Han, J. J.; Luo, Z. X.  
Charge transfer interactions of pyrazine with Ag-12 clusters towards precise SERS chemical mechanism  
Nanoscale, (10): 16787-16794. 2018. 10.1039/c8nr05253k

Anafcheh, M.; Naderi, F.  
The interaction of hydrogen with Li-coated C-70 fullerene: A DFT study  
International Journal of Hydrogen Energy, (43): 12271-12277. 2018.  
10.1016/j.ijhydene.2018.05.027

Anafcheh, M.; Naderi, F.; Ghafouri, R.  
Hydrogen-abstraction reactions of fully hydrogenated silicon fullerene cages with the amino radical: a density functional study  
Structural Chemistry, (29): 607-614. 2018. 10.1007/s11224-017-1057-1

Anafcheh, M.; Naderi, F.; Zahedi, M.  
Incorporation of topological defects and atomic impurities on the carbon nanotube surface: A DFT study of AD-dimer defects  
Heteroatom Chemistry, (29) 2018. 10.1002/hc.21431

Anastassova, N. O.; Mavrova, A. T.; Yancheva, D. Y.; Kondeva-Burdina, M. S.; Tzankova, V. I.; Stoyanov, S. S.; Shivachev, B. L.; Nikolova, R. P.  
Hepatotoxicity and antioxidant activity of some new N,N'-disubstituted benzimidazole-2-thiones, radical scavenging mechanism and structureactivity relationship  
Arabian Journal of Chemistry, (11): 353-369. 2018. 10.1016/j.arabjc.2016.12.003

Andrade, D. M.; Casals-Sainz, J. L.; Pendas, A. M.; Frenking, G.  
Dative and Electron-Sharing Bonding in C<sub>2</sub>F<sub>4</sub>  
Chemistry-a European Journal, (24): 9083-9089. 2018. 10.1002/chem.201800680

Andrella, N. O.; Liu, K. R.; Gabidullin, B.; Vasiliu, M.; Dixon, D. A.; Baker, R. T.  
Metal Heptafluoroisopropyl (M-hfip) Complexes for Use as hfip Transfer Agents  
Organometallics, (37): 422-432. 2018. 10.1021/acs.organomet.7b00837

Andrews, L.; Cho, H. G.; Fang, Z. T.; Vasiliu, M.; Dixon, D. A.

Tungsten Hydride Phosphorus- and Arsenic-Bearing Molecules with Double and Triple W-P and W-As Bonds

Inorganic Chemistry, (57): 5320-5332. 2018. 10.1021/acs.inorgchem.8b00348

Andrews, L.; Cho, H. G.; Gong, Y.

Reactions of Laser-Ablated Aluminum Atoms with Cyanogen: Matrix Infrared Spectra and Electronic Structure Calculations for Aluminum Isocyanides Al(NC)(1,2,3) and Their Novel Dimers

Journal of Physical Chemistry A, (122): 5342-5353. 2018. 10.1021/acs.jpca.8b02036

Andris, E.; Navratil, R.; Jasik, J.; Puri, M.; Costas, M.; Que, L.; Roithova, J.

Trapping Iron(III)-Oxo Species at the Boundary of the "Oxo Wall": Insights into the Nature of the Fe(III)-O Bond

Journal of the American Chemical Society, (140): 14391-14400. 2018. 10.1021/jacs.8b08950

Andris, E.; Navratil, R.; Jasik, J.; Sabanya, G.; Costas, M.; Srnec, M.; Roithova, J.

Detection of Indistinct Fe-N Stretching Bands in Iron(V) Nitrides by Photodissociation Spectroscopy

Chemistry-a European Journal, (24): 5078-5081. 2018. 10.1002/chem.201705307

Anglada, J. M.; Crehuet, R.; Adhikari, S.; Francisco, J. S.; Xia, Y.

Reactivity of hydopersulfides toward the hydroxyl radical unraveled: disulfide bond cleavage, hydrogen atom transfer, and proton-coupled electron transfer

Physical Chemistry Chemical Physics, (20): 4793-4804. 2018. 10.1039/c7cp07570g

Angnes, R. A.; Thompson, L. M.; Mashuta, M. S.; Correia, C. R. D.; Hammond, G. B.

Non-Covalent Substrate Directed Enantioselective Heck Desymmetrization of cis-Cyclohex-4-ene-1,2-diol: Synthesis of all cis Chiral 5-Aryl-cyclohex-3-ene-1,2-diols and Mechanistic Investigation

Advanced Synthesis & Catalysis, (360): 3760-3767. 2018. 10.1002/adsc.201800785

Anitha, K.; Balachandran, V.; Narayana, B.

Molecular orbital studies, frequency and solvent dependent NLO properties of (2E)-1-(4-bromophenyl)-3-(4-nitrophenyl) prop-2-en-1-one

Indian Journal of Pure & Applied Physics, (56): 91-107. 2018.

Annam, S.; Gopakumar, G.; Rao, C.; Sivaraman, N.; Sivaramakrishna, A.; Vijayakrishna, K.

Extraction of actinides by Tri-n-butyl phosphate derivatives: Effect of substituents

Inorganica Chimica Acta, (469): 123-132. 2018. 10.1016/j.ica.2017.07.048

Annam, S.; Gopakumar, G.; Rao, C.; Sivaraman, N.; Sivaramakrishna, A.; Vijayakrishna, K.

Trihexyl phosphate to trihexyl phosphine oxide: Diverse effect on extraction behavior of actinides

Journal of Molecular Liquids, (256): 416-423. 2018. 10.1016/j.molliq.2018.02.063

Ansari, S. A.; Mohapatra, P. K.; Ali, S. M.; Rawat, N.; Tomar, B. S.; Leoncini, A.; Huskens, J.; Verboom, W.

Complexation thermodynamics of tetraalkyl diglycolamides with trivalent f-elements in ionic liquids: spectroscopic, microcalorimetric and computational studies

New Journal of Chemistry, (42): 708-716. 2018. 10.1039/c7nj03925e

Anusha, C.; De, S.; Parameswaran, P.

Effect of Transition Metal Fragments on the Reverse Fritsch-Buttenberg-Wiechell Type Ring Contraction Reaction of Metallabenzenes to Metal-Carbene Complexes

Journal of Physical Chemistry A, (122): 2160-2167. 2018. 10.1021/acs.jpca.7b10335

Anusiewicz, I.; Skurski, P.

Attaching Be or Mg to BH<sub>3</sub> results in the formation of BeBH<sub>3</sub> and MgBH<sub>3</sub> molecules capable of forming stable anions

Chemical Physics Letters, (698): 19-23. 2018. 10.1016/j.cplett.2018.03.007

Aono, S.; Sakaki, S.

QM/MM Approach to Isomerization of Ruthenium(II) Sulfur Dioxide Complex in Crystal; Comparison with Solution and Gas Phases

Journal of Physical Chemistry C, (122): 20701-20716. 2018. 10.1021/acs.jpcc.8b04774

Arakawa, M.; Ando, K.; Fujimoto, S.; Mishra, S.; Patwari, G. N.; Terasaki, A.

The role of electronegativity on the extent of nitridation of group 5 metals as revealed by reactions of tantalum cluster cations with ammonia molecules

Physical Chemistry Chemical Physics, (20): 13974-13982. 2018. 10.1039/c8cp00424b

Ari, H.; Mihciokur, O.; Buyukmumcu, Z.; Mihciokur, H.; Ozpozan, T.

Electrochemical oligomerization of selenophene and band structure of polyselenophene: A density functional theory study

Computational Materials Science, (154): 65-74. 2018. 10.1016/j.commatsci.2018.07.025

Arioglu, C.; Tamer, O.; Avci, D.; Atalay, Y.

Optimized geometry, spectroscopic characterization and nonlinear optical properties of carbazole picrate: a density functional theory study

Indian Journal of Physics, (92): 1613-1621. 2018. 10.1007/s12648-018-1258-5

Aristizabal, L.; Angel, M.; Orozco, C.; Ruiz, P.; Quijano, J.; Notario, R.

Computational study of the thermal decomposition and the thermochemistry of allyl ethers and allyl sulfides

Structural Chemistry, (29): 897-907. 2018. 10.1007/s11224-018-1074-8

Arjunan, V.; Devi, L.; Mohan, S.

Conformational analysis, spectroscopic, structure-activity relations and quantum chemical simulation studies of 4-(trifluoromethyl) benzylamine

Journal of Molecular Structure, (1159): 103-117. 2018. 10.1016/j.molstruc.2018.01.049

- Arjunan, V.; Thirunarayanan, S.; Mohan, S.  
Energy profile, spectroscopic (FT-IR, FT-Raman and FT-NMR) and DFT studies of 4-bromoisophthalic acid  
*Journal of Molecular Structure*, (1157): 132-148. 2018. 10.1016/j.molstruc.2017.12.032
- Arkan, F.; Izadyar, M.  
Computational modeling of the photovoltaic activities in EABX(3) (EA = ethylammonium, B = Pb, Sn, Ge, X= Cl, Br, I) perovskite solar cells  
*Computational Materials Science*, (152): 324-330. 2018. 10.1016/j.commatsci.2018.06.006
- Arkan, F.; Izadyar, M.  
Molecular engineering of the organometallic perovskites/HTMs in the PSCs: Photovoltaic behavior and energy conversion  
*Solar Energy Materials and Solar Cells*, (180): 46-58. 2018. 10.1016/j.solmat.2018.02.021
- Arkan, F.; Izadyar, M.  
Recent theoretical progress in the organic/metal-organic sensitizers as the free dyes, dye/TiO<sub>2</sub> and dye/electrolyte systems; Structural modifications and solvent effects on their performance  
*Renewable & Sustainable Energy Reviews*, (94): 609-655. 2018. 10.1016/j.rser.2018.06.054
- Arora, R.; Kashyap, K.; Kakkar, R.  
Rearrangements in radical cations of diazoketones: A DFT mechanistic study  
*Computational and Theoretical Chemistry*, (1134): 30-36. 2018. 10.1016/j.comptc.2018.05.005
- Arslancan, S.; Lamsabhi, A.; Mo, O.; Yanez, M.  
Complexes between cyclopentene and cyclopentyne derivatives with HCu and FCu: The importance of cyclization effects  
*International Journal of Quantum Chemistry*, (118) 2018. 10.1002/qua.25489
- Asghar, A.; Raman, A. A. A.; Daud, W.; Ramalingam, A.  
Reactivity, stability, and thermodynamic feasibility of H<sub>2</sub>O<sub>2</sub>/H<sub>2</sub>O at graphite cathode: Application of quantum chemical calculations in MFCs  
*Environmental Progress & Sustainable Energy*, (37): 1291-1304. 2018. 10.1002/ep.12806
- Asghari, S.; Gouran, A. A.; Farmanzadeh, D.; Abdollahi, T.  
Investigating the reaction pathways of chemical functionalization of C-20 fullerene by nitrile oxide and azide: A computational study  
*Journal of Theoretical & Computational Chemistry*, (17) 2018. 10.1142/s0219633618500037
- Ashley, D. C.; Jakubikova, E.  
Tuning the Redox Potentials and Ligand Field Strength of Fe(II) Polypyridines: The Dual pi-Donor and pi-Acceptor Character of Bipyridine  
*Inorganic Chemistry*, (57): 9907-9917. 2018. 10.1021/acs.inorgchem.8b01002

- Asr, A.; Aghaie, M.; Emamian, S.; Aghaie, H.  
A molecular electron density theory study on the 3+2 cycloaddition reaction of thiocarbonyl ylides with hetaryl thioketones  
New Journal of Chemistry, (42): 11819-11830. 2018. 10.1039/c8nj02021c
- Asr, A.; Emamian, S.; Aghaie, M.; Aghaie, H.  
3+2 cycloaddition reaction between CF<sub>3</sub>-substituted thiocarbonyl ylides and thioketones: Exploration of regioselectivity and mechanistic aspects using Molecular Electron Density Theory  
Journal of Fluorine Chemistry, (209): 14-22. 2018. 10.1016/j.jfluchem.2018.02.006
- Astakhova, V. V.; Moskalik, M. Y.; Ganin, A. S.; Sterkhova, I. V.; Shainyan, B. A.  
Iodotriflamation vs. Electrophilic Aromatic Iodination in the Reaction of N-Phenyltriflamide with Alkenes  
Chemistryselect, (3): 5960-5964. 2018. 10.1002/slct.201801379
- Ates, O. D.; Zorlu, Y.; Kanmazalp, S. D.; Chumakov, Y.; Gurek, A. G.; Ayhan, M. M.  
Halogen bonding driven crystal engineering of iodophthalonitrile derivatives  
Crystengcomm, (20): 3858-3867. 2018. 10.1039/c8ce00594j
- Athar, M.; Das, S.; Jha, P. C.; Jha, A. M.  
Conformational equilibrium study of calix 4 tetrolarenes using Density Functional Theory (DFT) and Molecular Dynamics simulations  
Supramolecular Chemistry, (30): 982-993. 2018. 10.1080/10610278.2018.1517876
- Athar, M.; Lone, M. Y.; Jha, P. C.  
Recognition of anions using urea and thiourea substituted calixarenes: A density functional theory study of non-covalent interactions  
Chemical Physics, (501): 68-77. 2018. 10.1016/j.chemphys.2017.12.002
- Athare, S. V.; Gejji, S. P.  
Confinement of 1-butyl-3-methylimidazolium in cucurbiturils  
Journal of Molecular Liquids, (272): 496-506. 2018. 10.1016/j.molliq.2018.09.121
- Atilgan, A.; Yurdakul, S.; Erdogan, Y.; Gulluoglu, M. T.  
DFT simulation, quantum chemical electronic structure, spectroscopic and structure-activity investigations of 4-acetylpyridine  
Journal of Molecular Structure, (1161): 55-65. 2018. 10.1016/j.molstruc.2018.01.080
- Atim, S.; Yang, L.; Nesterov, V.; Wang, X. P.; Richmond, M. G.  
Synthesis of the labile rhenium(I) complexes fac-Re(CO)(3)(L) kappa(2)-O,O-FcC(O)CHC(O)Me (where Fc = ferrocenyl; L = THF, H<sub>2</sub>O, alkyne) and alkyne addition to the diketonate ligand  
Journal of Organometallic Chemistry, (874): 87-100. 2018. 10.1016/j.jorganchem.2018.06.005
- Attia, A. A. A.; Lulan, A.; King, R. B.

Polyhedral Trimetallaboranes of the Group 9 Metals: Isocloso versus Capped and Uncapped  
Closodeltahedra

Organometallics, (37): 1845-1851. 2018. 10.1021/acs.organomet.8b00077

Aurell, M. J.; Gonzalez-Cardenete, M. A.; Zaragoza, R. J.

A new mechanism for internal nucleophilic substitution reactions

Organic & Biomolecular Chemistry, (16): 1101-1112. 2018. 10.1039/c7ob02994b

Avci, D.; Alturk, S.; Sonmez, F.; Tamer, O.; Basoglu, A.; Atalay, Y.; Kurt, B. Z.; Dege, N.

Three novel Cu(II), Cd(II) and Cr(III) complexes of 6-Methylpyridine-2-carboxylic acid with thiocyanate: Synthesis, crystal structures, DFT calculations, molecular docking and alpha-Glucosidase inhibition studies

Tetrahedron, (74): 7198-7208. 2018. 10.1016/j.tet.2018.10.054

Avdeenko, A. P.; Konovalova, S. A.; Shishkina, S. V.

Activated Sterically Strained C=N Bond in N-Substituted p-Quinone Mono- and Diimines: XVI.  
Structural Characteristics

Russian Journal of Organic Chemistry, (54): 62-77. 2018. 10.1134/s1070428018010050

Avdovic, E. H.; Milenkovic, D.; Markovic, J. M. D.; Dorovic, J.; Vukovic, N.; Vukic, M. D.; Jevtic, V. V.;  
Trifunovic, S. R.; Potocnak, I.; Markovic, Z.

Synthesis, spectroscopic characterization (FT-IR, FT-Raman, and NMR), quantum chemical  
studies and molecular docking of 3-(1-(phenylamino)ethylidene)-chroman-2,4-dione

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (195): 31-40. 2018.  
10.1016/j.saa.2018.01.023

Avhad, K. C.; Patil, D. S.; Gawale, Y. K.; Chitrambalam, S.; Sreenath, M. C.; Joe, I. H.; Sekar, N.

Large Stokes Shifted Far-Red to NIR-Emitting D-pi-A Coumarins: Combined Synthesis,  
Experimental, and Computational Investigation of Spectroscopic and Non-Linear Optical Properties  
Chemistryselect, (3): 4393-4405. 2018. 10.1002/slct.201800063

Aviles-Moreno, J. R.; Berden, G.; Oomens, J.; Martinez-Haya, B.

Complexes of Crown Ether Macrocycles with Methyl Guanidinium: Insights into the Capture of  
Charge in Peptides

Chemphyschem, (19): 2169-2175. 2018. 10.1002/cphc.201800596

Aviles-Moreno, J. R.; Berden, G.; Oomens, J.; Martinez-Haya, B.

Guanidinium/ammonium competition and proton transfer in the interaction of the amino acid  
arginine with the tetracarboxylic 18-crown-6 ionophore

Physical Chemistry Chemical Physics, (20): 4067-4073. 2018. 10.1039/c7cp07975c

Aviles-Moreno, J. R.; Berden, G.; Oomens, J.; Martinez-Haya, B.

Intra-cavity proton bonding and anharmonicity in the anionophore cyclen

Physical Chemistry Chemical Physics, (20): 8968-8975. 2018. 10.1039/c8cp00660a

Awad, M. K.; Abdel-Aal, M. F.; Atlam, F. M.; Hekal, H. A.

Design, synthesis, molecular modeling, and biological evaluation of novel alpha-aminophosphonates based quinazolinone moiety as potential anticancer agents: DFT, NBO and vibrational studies

Journal of Molecular Structure, (1173): 128-141. 2018. 10.1016/j.molstruc.2018.06.094

Awad, M. K.; Abdel-Aal, M. F.; Atlam, F. M.; Hekal, H. A.

Synthesis of New alpha-Amino Phosphonates Containing 3-Amino-4(3H) Quinazolinone Moiety as Anticancer and Antimicrobial Agents: DFT, NBO, and Vibrational Studies

Current Organic Synthesis, (15): 286-296. 2018. 10.2174/1570179414666170703141629

Azharhazin, E.; Izadyar, M.; Housaindokht, M. R.

Molecular dynamic simulation and DFT study on the Drug-DNA interaction; Crocetin as an anti-cancer and DNA nanostructure model

Journal of Biomolecular Structure & Dynamics, (36): 1063-1074. 2018.

10.1080/07391102.2017.1310060

Aziz, S. G.; Osman, O. I.; Elroby, S. A.; Hassan, W. M. I.; Jedidi, A.; Hilal, R. H.

Proton-coupled electron transfer in dye-sensitized solar cells: a theoretical perspective

Structural Chemistry, (29): 983-997. 2018. 10.1007/s11224-018-1080-x

Badhani, B.; Kakkar, R.

Structural, electronic, and reactivity parameters of some triorganotin(IV) carboxylates: a DFT analysis

Structural Chemistry, (29): 753-763. 2018. 10.1007/s11224-017-1068-y

Badr, E. A.; Bedair, M. A.; Shaban, S. M.

Adsorption and performance assessment of some imine derivatives as mild steel corrosion inhibitors in 1.0 M HCl solution by chemical, electrochemical and computational methods

Materials Chemistry and Physics, (219): 444-460. 2018. 10.1016/j.matchemphys.2018.08.041

Baei, M. T.; Koohi, M.; Shariati, M.

Characterization of C-20 fullerene and its isolated C<sub>20</sub>-nGen derivatives (n=1-5) by alternating germanium atom(s) in equatorial position: A DFT survey

Heteroatom Chemistry, (29) 2018. 10.1002/hc.21410

Baei, M. T.; Koohi, M.; Shariati, M.

Structure, stability, and electronic properties of AlP nanocages evolved from the world's smallest caged fullerene C-20: A computational study at DFT

Journal of Molecular Structure, (1159): 118-134. 2018. 10.1016/j.molstruc.2018.01.022

Baez-Grez, R.; Ruiz, L.; Pino-Rios, R.; Tiznado, W.

Which NICS method is most consistent with ring current analysis? Assessment in simple monocycles

RSC Advances, (8): 13446-13453. 2018. 10.1039/c8ra01263f

Baggioli, A.

Noncovalent Interactions Descriptor Based on the Source Function of Individual Localized Molecular Orbitals in Whole Space

Journal of Physical Chemistry A, (122): 3850-3857. 2018. 10.1021/acs.jpca.7608774

Bahri-Laleh, N.; Hanifpour, A.; Mirmohammadi, S. A.; Poater, A.; Nekoomanesh-Haghghi, M.; Talarico, G.; Cavallo, L.

Computational modeling of heterogeneous Ziegler-Natta catalysts for olefins polymerization  
Progress in Polymer Science, (84): 89-114. 2018. 10.1016/j.progpolymsci.2018.06.005

Bai, H. N.; Xu, H.; Zhang, H. M.; Guo, Y.; Shan, J. K.; Wei, D. H.; Zhu, Y. Y.; Zhang, S. R.; Zhang, W. J.

Theoretical investigations of the Ir-catalyzed direct borylation of B(3,6)-H of o-carborane: the actual catalyst, mechanism, and origin of regioselectivity

Catalysis Science & Technology, (8): 5165-5177. 2018. 10.1039/c8cy01322e

Bailey, G. A.; Foscato, M.; Higman, C. S.; Day, C. S.; Jensen, V. R.; Fogg, D. E.

Bimolecular Coupling as a Vector for Decomposition of Fast-Initiating Olefin Metathesis Catalysts

Journal of the American Chemical Society, (140): 6931-6944. 2018. 10.1021/jacs.8b02709

Bakic, M. T.; Cetina, M.; Mazalovic, S.

Molecular structure of a tolyl derivative of gamma-pyrone

Journal of Molecular Structure, (1151): 256-265. 2018. 10.1016/j.molstruc.2017.09.050

Bakic, M. T.; Nuskol, M.; Mikac, L.

Structural and Spectroscopic Properties of 2-Bromoacetyl naphthalene: Experimental and Computational (DFT) Analysis

Chemistryselect, (3): 4185-4199. 2018. 10.1002/slct.201800282

Bakthavachalam, K.; Dutta, S.; Arivazhagan, C.; Raghavendra, B.; Haridas, A.; Sen, S. S.; Koley, D.; Ghosh, S.

Cyclometallation of a germylene ligand by concerted metalation-deprotonation of a methyl group

Dalton Transactions, (47): 15835-15844. 2018. 10.1039/c8dt03166e

Balaeff, A.; Kuznetsov, A. E.

Three Ligands with Biomedical Importance: Binding to Small ZnS Quantum Dots

Journal of Physical Chemistry C, (122): 12454-12463. 2018. 10.1021/acs.jpcc.8b00936

Banerjee, P.; Chakraborty, T.

Weak hydrogen bonds: insights from vibrational spectroscopic studies  
International Reviews in Physical Chemistry, (37): 83-123. 2018.

10.1080/0144235x.2018.1419731

Banerjee, S.; Sreenithya, A.; Sunoj, R. B.

Machine learning for predicting product distributions in catalytic regioselective reactions  
Physical Chemistry Chemical Physics, (20): 18311-18318. 2018. 10.1039/c8cp03141j

Barama, L.; Bayoud, B.; Chafaa, F.; Nacereddine, A. K.; Djerourou, A.

A mechanistic MEDT study of the competitive catalysed 4+2 and 2+2 cycloaddition reactions between 1-methyl-1-phenylallene and methyl acrylate: the role of Lewis acid on the mechanism and selectivity

Structural Chemistry, (29): 1709-1721. 2018. 10.1007/s11224-018-1152-y

Baranac-Stojanovic, M.

Can Variations of (<sup>1</sup>H-NMR)-H-1 Chemical Shifts in Benzene Substituted with an Electron-Accepting (NO<sub>2</sub>)/Donating (NH<sub>2</sub>) Group be Explained in Terms of Resonance Effects of Substituents?  
Chemistry-an Asian Journal, (13): 877-881. 2018. 10.1002/asia.201800137

Barati-darband, F.; Izadyar, M.; Arkan, F.

Anchoring Group and a pi-Spacer Effects on the Dynamics and Kinetics of the Photovoltaic Processes in the Quinoxaline-Based Organic Dye-Sensitized Solar Cells  
Journal of Physical Chemistry C, (122): 23968-23977. 2018. 10.1021/acs.jpcc.8b07965

Barbosa, T. M.; Viesser, R. V.; Martins, L. G.; Rittner, R.; Tormena, C. F.

The Antagonist Effect of Nitrogen Lone Pair: (3)J(HF) versus (5)J(HF)  
Chemphyschem, (19): 1358-1362. 2018. 10.1002/cphc.201800073

Barrales-Martinez, C.; Cortes-Arriagada, D.; Gutierrez-Oliva, S.

Molecular hydrogen formation in the interstellar medium: the role of polycyclic aromatic hydrocarbons analysed by the reaction force and activation strain model

Monthly Notices of the Royal Astronomical Society, (481): 3052-3062. 2018.

10.1093/mnras/sty2215

Barroso, J.; Murillo, F.; Martinez-Guajardo, G.; Ortiz-Chi, F.; Pan, S.; Fernandez-Herrera, M. A.; Merino, G.

Bonding and Mobility of Alkali Metals in Helicenes

Chemistry-a European Journal, (24): 11227-11233. 2018. 10.1002/chem.201802222

Bassou, D.; Ghomri, A.; Atmani, A.

Reactivity of beta-substituted phosphoenol pyruvates towards alkoxides: a theoretical and experimental study

Progress in Reaction Kinetics and Mechanism, (43): 211-218. 2018.

10.3184/146867818x15161889114466

Bauza, A.; Quinonero, D.; Frontera, A.  
Substituent Effects in Multivalent Halogen Bonding Complexes: A Combined Theoretical and Crystallographic Study  
*Molecules*, (23) 2018. 10.3390/molecules23010018

Bayse, C. A.  
Halogen bonding from the bonding perspective with considerations for mechanisms of thyroid hormone activation and inhibition  
*New Journal of Chemistry*, (42): 10623-10632. 2018. 10.1039/c8nj00737c

Bazargan, G.; Sohlberg, K.  
Advances in modelling switchable mechanically interlocked molecular architectures  
*International Reviews in Physical Chemistry*, (37): 1-82. 2018. 10.1080/0144235x.2018.1419042

Bazel, Y.; Leskova, M.; Reclo, M.; Sandrejova, J.; Simon, A.; Fizer, M.; Sidey, V.  
Structural and spectrophotometric characterization of 2- 4-4(dimethylamino)styryl -1-ethylquinolinium iodide as a reagent for sequential injection determination of tungsten  
*Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy*, (196): 398-405. 2018. 10.1016/j.saa.2018.02.049

Beaula, T. J.; Muthuraja, P.; Dhandapani, M.; Jothy, V. B.  
Effect of charge transfer with spectral analysis on the antibacterial compound 4-(Dimethyl amino) pyridine: 3,5-Dinitrobenzoic acid: Experimental and theoretical perspective  
*Journal of Molecular Structure*, (1171): 511-526. 2018. 10.1016/j.molstruc.2018.06.026

Behjatmanesh-Ardakani, R.  
Periodic and non-periodic DFT modeling of CO reduction on the surface of Ni-doped graphene nanosheet  
*Molecular Catalysis*, (455): 239-249. 2018. 10.1016/j.mcat.2018.06.008

Belogolova, E. F.; Doronina, E. P.; Sidorkin, V. F.  
Assignment of photoelectron spectra of intramolecular silicon complexes: 1-vinyl- and 1-phenylsilatrane  
*Physical Chemistry Chemical Physics*, (20): 26210-26220. 2018. 10.1039/c8cp04582h

Belostotskii, A. M.  
Nanosecond-Scale Isomerization of the 4'-Carboxonium Cation Oxidatively Produced in Pyrimidine Units of DNA  
*Journal of Organic Chemistry*, (83): 11604-11613. 2018. 10.1021/acs.joc.8b01580

Belova, N. V.; Girichev, G. V.; Kotova, V. E.; Korolkova, K. A.; Trang, N. H.  
The molecular structure of 4-methylpyridine-N-oxide: Gas-phase electron diffraction and quantum chemical calculations  
*Journal of Molecular Structure*, (1156): 210-215. 2018. 10.1016/j.molstruc.2017.11.070

Belyakov, A. V.; Nikolaenko, K. O.; Davidovich, P. B.; Ivanov, A. D.; Ponyaev, A. I.; Rykov, A. N.; Shishkov, I. F.

The molecular structure of 5-X-isatines where (X = F, Cl, and Br) determined by gas-phase electron diffraction with theoretical calculations

Journal of Molecular Structure, (1152): 361-367. 2018. 10.1016/j.molstruc.2017.09.117

Ben El Ayouchia, H.; Bahsis, L.; Anane, H.; Domingo, L. R.; Stiriba, S. E.

Understanding the mechanism and regioselectivity of the copper(I) catalyzed 3+2 cycloaddition reaction between azide and alkyne: a systematic DFT study

RSC Advances, (8): 7670-7678. 2018. 10.1039/c7ra10653j

Ben Issa, T.; Hassine, C. B.; Ghalla, H.; Barhoumi, H.; Benhamada, L.

Experimental and computational study of electronic, electrochemical and thermal properties of quinoline phosphate

Journal of Molecular Structure, (1162): 71-80. 2018. 10.1016/j.molstruc.2018.02.085

Benallou, A.

An investigation of molecular mechanism and the role of Te-bridged-atom in the formation of polysubstituted pyridines via Hetero-Diels-Alder reaction of isotellurazole with acetylenic dienophile: a molecular electron density study

Journal of Chemical Sciences, (130) 2018. 10.1007/s12039-018-1459-7

Bende, A.; Gaele, M. F.; Di Palma, T. M.

UV Photoionization of Sodium-Doped Formic Acid Clusters

Chemphyschem, (19): 2724-2734. 2018. 10.1002/cphc.201800507

Benhassine, A.; Boulebd, H.; Anak, B.; Bouraiou, A.; Bouacida, S.; Bencharif, M.; Belfaitah, A.

Cobalt(II) complexes based on (1-methyl-1H-benzo d imidazol-2-yl) methanol derivative: synthesis, crystal structure, spectroscopy, DFT calculations, and antioxidant activity

Journal of Coordination Chemistry, (71): 311-328. 2018. 10.1080/00958972.2018.1428742

Benhassine, A.; Boulebd, H.; Anak, B.; Bouraiou, A.; Bouacida, S.; Bencharif, M.; Belfaitah, A.

Copper(II) and zinc(II) as metal-carboxylate coordination complexes based on (1-methyl-1H-benzo d imidazol-2-yl) methanol derivative: Synthesis, crystal structure, spectroscopy, DFT calculations and antioxidant activity

Journal of Molecular Structure, (1160): 406-414. 2018. 10.1016/j.molstruc.2018.02.033

BenNasr, F.; Perez-Mellor, A.; Alata, I.; Lepere, V.; Jaidane, N. E.; Zehnacker, A.

Stereochemistry-dependent hydrogen bonds stabilise stacked conformations in jet-cooled cyclic dipeptides: (LD) vs. (LL) cyclo tyrosine-tyrosine

Faraday Discussions, (212): 399-419. 2018. 10.1039/c8fd00079d

Bernhard, D.; Dietrich, F.; Fatima, M.; Perez, C.; Gottschalk, H. C.; Wuttke, A.; Mata, R. A.; Suhm, M. A.; Schnell, M.; Gerhards, M.

The phenyl vinyl ether-methanol complex: a model system for quantum chemistry benchmarking

Beilstein Journal of Organic Chemistry, (14): 1642-1654. 2018. 10.3762/bjoc.14.140

Beyramabadi, S. A.; Javan-Khoshkholgh, M.; Ostad, N. J.; Gharib, A.; Ramezanadeh, M.; Sadeghi, M.; Bazian, A.; Morsali, A.

Spectroscopic (Ft-Ir, Nmr, Uv-Vis, Fluorescence) and Dft Studies (Molecular Structure, Ir and Nmr Spectral Assignments, Nbo and Fukui Function) of Schiff Bases Derived from 2-Chloro-3-Quinolinecarboxaldehyde

Journal of Structural Chemistry, (59): 1342-1352. 2018. 10.1134/s0022476618060136

Beyzaei, H.; Baranipour, P.; Aryan, R.; Karimi, P.; Sanchooli, M.; Delarami, H. S.

Multicomponent Solvent-Free Synthesis, Antibacterial Evaluation and QSAR Study of 2-(Bis(benzylthio)methylene)malononitriles

Acta Chimica Slovenica, (65): 757-767. 2018. 10.17344/acsi.2018.4621

Bhai, S.; Jana, K.; Ganguly, B.

Probing the Structural and Electronic Effects on the Origin of pi-Facial Stereoselectivity in 1-Methylphosphole 1-Oxide Cycloadditions and Cyclodimerization

ACS Omega, (3): 10945-10952. 2018. 10.1021/acsomega.8b01165

Bharadwaz, P.; Dewhurst, R. D.; Phukan, A. K.

Metal-Free Activation of Enthalpically Strong Bonds: Unraveling the Potential of Hitherto Unexplored Singlet Carbenes

Advanced Synthesis & Catalysis, (360): 4543-4561. 2018. 10.1002/adsc.201800873

Bhat, R. A.; Kumar, D.; Alam, A.; Mir, B. A.; Srivastava, A.; Malla, M. A.; Mir, M. A.

Synthesis, characterization, thermal and DFT studies of S-methyl-beta-N(3-(2-nitrophenyl)allylidene)dithiocarbazate as anti-bacterial agent

Journal of Molecular Structure, (1173): 72-80. 2018. 10.1016/j.molstruc.2018.06.061

Bhat, R. A.; Kumar, D.; Malla, M. A.; Bhat, S. U.; Khan, M. S.; Manzoor, O.; Srivastava, A.; Naikoo, R. A.; Mohsin, M.; Mir, M. A.

Synthesis, characterization, computational studies and biological evaluation of S-benzyl-beta-N-3-(4-hydroxy-3-methoxy-phenylallylidene) dithiocarbazate

Journal of Molecular Structure, (1156): 280-289. 2018. 10.1016/j.molstruc.2017.11.051

Bhat, R. A.; Kumar, D.; Srivastava, A.; Mir, B. A.; Malla, M. A.; Bhat, M. A.; Mir, M. A.

Experimental, DFT Studies and Biological Evaluation of S-methyl-beta-N-(3-(2-nitrophenyl)allylidene)dithiocarbazate

Chemistryselect, (3): 7363-7369. 2018. 10.1002/slct.201801698

Bhattacharjee, I.; Acharya, N.; Karmakar, S.; Ray, D.

Room-Temperature Orange-Red Phosphorescence by Way of Intermolecular Charge Transfer in Single-Component Phenoxazine-Quinoline Conjugates and Chemical Sensing

Journal of Physical Chemistry C, (122): 21589-21597. 2018. 10.1021/acs.jpcc.8b06171

Bhattacharjee, I.; Ghosh, N.; Raina, A.; Dasgupta, J.; Ray, D.

Conformational switching via an intramolecular H-bond modulates the fluorescence lifetime in a novel coumarin-imidazole conjugate

Physical Chemistry Chemical Physics, (20): 6060-6072. 2018. 10.1039/c7cp07274k

Bhattacharyya, A.; Leoncini, A.; Egberink, R. J. M.; Mohapatra, P. K.; Verma, P. K.; Kanekar, A. S.; Yadav, A. K.; Jha, S. N.; Bhattacharyya, D.; Huskens, J.; Verboom, W.

First Report on the Complexation of Actinides and Lanthanides Using 2,2'-2"-(((1,4,7-Triazonane-1,4,7-triyl)tris(2-oxoethane-2,1-diyl)) tris(oxy)) tris(N,N-diethylacetamide): Synthesis, Extraction, Luminescence, EXAFS, and DFT Studies

Inorganic Chemistry, (57): 12987-12998. 2018. 10.1021/acs.inorgchem.8b02255

Bhattacharyya, A.; Mohapatra, P. K.; Raut, D. R.; Leoncini, A.; Huskens, J.; Verboom, W.

Unusual Reversal in Pu and U Extraction in an Ionic Liquid Using Two Tripodal Diglycolamide Ligands: Experimental and DFT Studies

Solvent Extraction and Ion Exchange, (36): 542-557. 2018. 10.1080/07366299.2018.1545285

Bhattacharyya, M.; Yuvaraj, K.; Chanda, A.; Ramkumar, V.; Ghosh, S.

Metal-Rich Metallaboranes: Structures and Geometries of Heterometallic mu(9)-Boride Clusters  
European Journal of Inorganic Chemistry: 2574-2583. 2018. 10.1002/ejic.201800375

Bhunia, S.; Kumar, A.; Singh, A.; Ojha, A. K.

Binding patterns of metal cations (Na<sup>+</sup>, K, Cu<sup>2+</sup>, and Zn<sup>2+</sup>) with Trp-Trp di-peptide investigated by DFT, NBO, and MD simulation

Computational and Theoretical Chemistry, (1141): 7-14. 2018. 10.1016/j.comptc.2018.08.010

Bhuvaneswari, G.; Prasad, L. G.; Prabavathi, N.

Crystal growth, experimental and theoretical investigations of organic NLO material 4-nitrophthalimide

Optik, (166): 307-316. 2018. 10.1016/j.ijleo.2018.03.129

Bhuvaneswari, G.; Prasad, L. G.; Prabhavathi, N.

Structural, optical, thermal and theoretical investigations on high efficiency NLO crystal: 4-Nitrobenzonitrile

Optik, (157): 1078-1086. 2018. 10.1016/j.ijleo.2017.11.194

Bhuvaneswari, R.; Bharathi, M. D.; Anbalagan, G.; Chakkavarthi, G.; Murugesan, K. S.

Molecular structure, vibrational spectroscopic (FT-IR, FT-Raman), NBO, HOMO and LUMO analysis of morpholinium oxalate by density functional method

Journal of Molecular Structure, (1173): 188-195. 2018. 10.1016/j.molstruc.2018.06.109

Bichan, N. G.; Ovchenkova, E. N.; Kudryakova, N. O.; Ksenofontov, A. A.; Gruzdev, M. S.; Lomova, T. N.  
Self-assembled cobalt(II)porphyrin-fulleropyrrolidine triads via axial coordination with  
photoinduced electron transfer

New Journal of Chemistry, (42): 12449-12456. 2018. 10.1039/c8nj00887f

Bilge, M.

A Dft Investigation of the Interaction of B- And Al-Doped C-60 Fullerenes with  
Cyclopropylpipezarine

Journal of Structural Chemistry, (59): 1271-1275. 2018. 10.1134/s0022476618060045

Bin, L.; Zhao, G. M.; Guo, X. J.

Theoretical investigation into the cooperativity effect and thermodynamic property of beta-nitroguanidine center dot C2F4 center dot H2O ternary complex

Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (57): 150-162. 2018.

Binder, J. F.; Kosnik, S. C.; Macdonald, C. L. B.

Assessing the Ligand Properties of NHC-Stabilised Phosphorus(I) Cations  
Chemistry-a European Journal, (24): 3556-3565. 2018. 10.1002/chem.201705224

Binder, J. F.; Swidan, A.; Macdonald, C. L. B.

Synthesis of Heteroleptic Phosphorus(I) Cations by P+ Transfer  
Inorganic Chemistry, (57): 11717-11725. 2018. 10.1021/acs.inorgchem.8b01822

Binh, D. H.; Hamdaoui, M.; Fischer-Krauser, D.; Karmazin, L.; Bailly, C.; Djukic, J. P.

Entrapment of THF-Stabilized Iridacyclic Ir-III Silylenes from Double H-Si Bond Activation and H-2 Elimination

Chemistry-a European Journal, (24): 17577-17589. 2018. 10.1002/chem.201804048

Biswas, S.; Pramanik, A.; Sarkar, P.

Computational Design of Quaterpyridine-Based Fe/Mn-Complexes for the Direct Hydrogenation of CO2 to HCOOH: A Direction for Atom-Economic Approach

Chemistryselect, (3): 5185-5193. 2018. 10.1002/slct.201800169

Blackaby, W. J. M.; Sabater, S.; Poulten, R. C.; Page, M. J.; Folli, A.; Krewald, V.; Mahon, M. F.; Murphy, D. M.; Richards, E.; Whittlesey, M. K.

Mono- and dinuclear Ni(I) products formed upon bromide abstraction from the Ni(I) ring-expanded NHC complex Ni(6-Mes)(PPh<sub>3</sub>)Br

Dalton Transactions, (47): 769-782. 2018. 10.1039/c7dt04187j

Blanco, S.; Lopez, J. C.

Rotational Characterization of an n -> pi\* Interaction in a Pyridine-Formaldehyde Adduct

Journal of Physical Chemistry Letters, (9): 4632-4637. 2018. 10.1021/acs.jpclett.8b01719

Bleiziffer, P.; Schaller, K.; Riniker, S.

Machine Learning of Partial Charges Derived from High-Quality Quantum-Mechanical Calculations

Journal of Chemical Information and Modeling, (58): 579-590. 2018. 10.1021/acs.jcim.7b00663

Blum, M.; Gebhardt, J.; Papendick, M.; Schlindwein, S. H.; Nieger, M.; Gudat, D.

Coordination isomerism in N-heterocyclic phosphonium thiocyanates

Canadian Journal of Chemistry, (96): 549-554. 2018. 10.1139/cjc-2017-0647

Blum, M.; Kappler, J.; Schlindwein, S. H.; Nieger, M.; Gudat, D.

Synthesis, spectroscopic characterisation and transmetalation of lithium and potassium diaminophosphanide-boranes

Dalton Transactions, (47): 112-119. 2018. 10.1039/c7dt04110a

Bobbitt, N. S.; Snurr, R. Q.

Competitive Adsorption of Methyl Bromide and Water on Metal Catecholates: Insights from Density Functional Theory

Industrial & Engineering Chemistry Research, (57): 17488-17495. 2018.

10.1021/acs.iecr.8b04377

Bohme, M.; Ziegenbalg, S.; Aliabadi, A.; Schnegg, A.; Gorls, H.; Plass, W.

Magnetic relaxation in cobalt( II)- based single- ion magnets influenced by distortion of the pseudotetrahedral N<sub>2</sub>O<sub>2</sub> coordination environment

Dalton Transactions, (47) 2018. 10.1039/c8dt01530a

Bohnke, J.; Dellermann, T.; Celik, M. A.; Krummenacher, I.; Dewhurst, R. D.; Demeshko, S.; Ewing, W. C.; Hammond, K.; Hess, M.; Bill, E.; Welz, E.; Rohr, M. I.; Mitric, R.; Engels, B.; Meyer, F.; Braunschweig, H.

Isolation of diborenes and their 90 degrees-twisted diradical congeners

Nature Communications, (9) 2018. 10.1038/s41467-018-02998-3

Bonyhady, S. J.; DeRosha, D. E.; Vela, J.; Vinyard, D. J.; Cowley, R. E.; Mercado, B. Q.; Brennessel, W. W.; Holland, P. L.

Iron and Cobalt Diazoalkane Complexes Supported by beta-Diketiminate Ligands: A Synthetic, Spectroscopic, and Computational Investigation

Inorganic Chemistry, (57): 5959-5972. 2018. 10.1021/acs.inorgchem.8b00468

Borah, M. M.; Devi, T. G.

The vibrational spectroscopic studies and molecular property analysis of Estradiol, Tamoxifen and their interaction by density functional theory

Journal of Molecular Structure, (1163): 205-220. 2018. 10.1016/j.molstruc.2018.02.096

Borah, M. M.; Devi, T. G.

Vibrational study and Natural Bond Orbital analysis of serotonin in monomer and dimer states by density functional theory

Journal of Molecular Structure, (1161): 464-476. 2018. 10.1016/j.molstruc.2018.02.055

Borgohain, R.; Handique, J. G.; Guha, A. K.; Pratihar, S.

A theoretical study of antioxidant activity of some Schiff bases derived from biologically important phenolic aldehydes and phenylenediamines

Journal of Physical Organic Chemistry, (31) 2018. 10.1002/poc.3757

Borosky, G. L.; Stavber, S.; Laali, K. K.

Iodine Activation of Alcohols: A Computational Study

Topics in Catalysis, (61): 636-642. 2018. 10.1007/s11244-018-0918-1

Boruah, A.; Borpuzari, M. P.; Maity, R.; Kar, R.

Iron sandwiched between group 13 analogues of N-Heterocyclic carbene: A theoretical investigation

Journal of Organometallic Chemistry, (863): 54-59. 2018. 10.1016/j.jorgancem.2018.03.028

Boshkow, J.; Scattolin, T.; Schoenebeck, F.; Carreira, E. M.

1,3 -Sigmatropic Shift of an Allylic Chloride

Helvetica Chimica Acta, (101) 2018. 10.1002/hlca.201800148

Bouchoucha, A.; Zaater, S.; Bouacida, S.; Merazig, H.; Djabbar, S.

Synthesis and characterization of new complexes of nickel (II), palladium (II) and platinum(II) with derived sulfonamide ligand: Structure, DFT study, antibacterial and cytotoxicity activities

Journal of Molecular Structure, (1161): 345-355. 2018. 10.1016/j.molstruc.2018.02.057

Bouska, M.; Tydlitat, J.; Jirasko, R.; Ruzicka, A.; Dostal, L.; Herres-Pawlis, S.; Hoffmann, A.; Jambor, R.

Reactivity of a NSn Coordinated Distannyne: Reduction and Hydrogen Abstraction

European Journal of Inorganic Chemistry: 2038-2044. 2018. 10.1002/ejic.201800370

Bouzayani, N.; Marque, S.; Djelassi, B.; Kacem, Y.; Marrot, J.; Ben Hassine, B.

Enantiopure Schiff bases of amino acid phenylhydrazides: impact of the hydrazide function on their structures and properties

New Journal of Chemistry, (42): 6389-6398. 2018. 10.1039/c7nj04597b

Bowman, M. C.; Burke, A. D.; Turney, J. M.; Schaefer, H. F.

Mechanisms of the Ethynyl Radical Reaction with Molecular Oxygen

Journal of Physical Chemistry A, (122): 9498-9511. 2018. 10.1021/acs.jpca.8b09862

Boyde, N. C.; Steelman, G. W.; Hanusa, T. P.

Multicomponent Mechanochemical Synthesis of Cyclopentadienyl Titanium tert-Butoxy Halides,  $CpxTiXy((OBu)-Bu-t)(4-(x+y))$  ( $x, y = 1, 2; X = Cl, Br$ )

ACS Omega, (3): 8149-8159. 2018. 10.1021/acsomega.8b00943

Boyle, T. J.; Perales, D.; Rimsza, J. M.; Alam, T. M.; Boye, D. M.; Sears, J. M.; Greathouse, J. A.; Kemp, R. A.

Synthesis and characterization of thallium-salen derivatives for use as underground fluid flow tracers

Dalton Transactions, (47): 4162-4174. 2018. 10.1039/c7dt04121g

Boz, E.; Tuzun, N. S.; Stein, M.

Computational investigation of the control of the thermodynamics and microkinetics of the reductive amination reaction by solvent coordination and a co-catalyst

RSC Advances, (8): 36662-36674. 2018. 10.1039/c8ra08135b

Bragiel, P.; Radkowska, I.; Belka, R.; Marciniak, B.; Bak, Z.

Structural, spectroscopic and NLO features of the 4-chloro-1-naphthol

Journal of Molecular Structure, (1154): 27-38. 2018. 10.1016/j.molstruc.2017.10.017

Brand, S.; Elsen, H.; Langer, J.; Donaubauer, W. A.; Hampel, F.; Harder, S.

Facile Benzene Reduction by a Ca<sup>2+</sup>/Al-I Lewis Acid/Base Combination

Angewandte Chemie-International Edition, (57): 14169-14173. 2018. 10.1002/anie.201809236

Brazon, E. A. M.; Flores-Sumozza, M. C.; Gomez, E. C.; Puello-Polo, E.

Study of the Influence of the polarization of the neighboring group C = X, in the kinetics of hydrogen chloride removal from beta- (substituted) alkyl chlorides (X = CH<sub>2</sub> S, NH, PH), using the density functional theory

Afinidad, (75): 52-60. 2018.

Brea, O.; Corral, I.

Super Strong Be-Be Bonds: Theoretical Insight into the Electronic Structure of Be-Be Complexes with Radical Ligands

Journal of Physical Chemistry A, (122): 2258-2265. 2018. 10.1021/acs.jpca.7b11758

Brea, O.; Luna, A.; Diaz, C.; Corral, I.

Molecular Modelling of the H-2-Adsorptive Properties of Tetrazolate-Based Metal-Organic Frameworks: From the Cluster Approach to Periodic Simulations

Chemphyschem, (19): 1349-1357. 2018. 10.1002/cphc.201800077

Brea, O.; Mo, O.; Yanez, M.; Montero-Campillo, M. M.; Alkorta, I.; Elguero, J.

Are beryllium-containing biphenyl derivatives efficient anion sponges?

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-017-3551-1

Bresien, J.; Hering-Junghans, C.; Kumm, P.; Schulz, A.; Thomas, M.; Villinger, A.

Dispersion Makes a Difference - The Solid-State Structure of Hg N(SiMe<sub>3</sub>)<sub>2</sub>(2)

European Journal of Inorganic Chemistry: 647-651. 2018. 10.1002/ejic.201701331

Bresien, J.; Hering-Junghans, C.; Schulz, A.; Thomas, M.; Villinger, A.  
Reactivity of TerN(SiMe<sub>3</sub>)BiCl<sub>2</sub>-Synthesis of an Aminobismuthenium Cation and  
TerN(SiMe<sub>3</sub>)Bi(N-3)(2)  
*Organometallics*, (37): 2571-2580. 2018. 10.1021/acs.organomet.8b00318

Bresien, J.; Hinz, A.; Schulz, A.; Villinger, A.  
Trapping of transient, heavy pnictogen-centred biradicals  
*Dalton Transactions*, (47): 4433-4436. 2018. 10.1039/c8dt00487k

Breton, G. W.  
DFT study of ortho, meta and para-pyridyl cations. Pyridinium found?  
*Computational and Theoretical Chemistry*, (1133): 51-57. 2018. 10.1016/j.comptc.2018.04.013

Breugst, M.; Huisgen, R.; Reissig, H. U.  
Regioselective 1,3-Dipolar Cycloadditions of Diazoalkanes with Heteroatom-Substituted Alkynes:  
Theory and Experiment  
*European Journal of Organic Chemistry*: 2477-2485. 2018. 10.1002/ejoc.201800100

Brovarets, O. O.; Voiteshenko, I. S.; Perez-Sanchez, H.; Hovorun, D. M.  
A QM/QTAIM detailed look at the Watson-Crick <-> wobble tautomeric transformations of the  
2-aminopurine.pyrimidine mispairs  
*Journal of Biomolecular Structure & Dynamics*, (36): 1649-1665. 2018.  
10.1080/07391102.2017.1331864

Brugos, J.; Cabeza, J. A.; Garcia-Alvarez, P.; Perez-Carreno, E.  
From a PGeP Pincer-Type Germylene to Metal Complexes Featuring Chelating (Ir) and Tripodal  
(Ir) PGeP Germyl and Bridging (Mn-2) and Chelating (Ru) PGeP Germylene Ligands  
*Organometallics*, (37): 1507-1514. 2018. 10.1021/acs.organomet.8b00171

Brugos, J.; Cabeza, J. A.; Garcia-Alvarez, P.; Perez-Carreno, E.; Polo, D.  
Synthesis and some coordination chemistry of the PSnP pincer-type stannylene  
Sn(NCH<sub>2</sub>PtBu<sub>2</sub>)(2)C<sub>6</sub>H<sub>4</sub>, attempts to prepare the PSiP analogue, and the effect of the E atom on the  
molecular structures of E(NCH<sub>2</sub>PtBu<sub>2</sub>)(2)C<sub>6</sub>H<sub>4</sub> (E = C, Si, Ge, Sn)  
*Dalton Transactions*, (47): 4534-4544. 2018. 10.1039/c7dt04561a

Brzeski, J.; Anusiewicz, I.; Skurski, P.  
The acid strength of the HClO<sub>4</sub>/n(AlF<sub>3</sub>) and HClO<sub>4</sub>/n(SbF<sub>5</sub>) (n=1-3) Lewis-Bronsted superacids  
containing the excess of the Lewis acid component  
*Theoretical Chemistry Accounts*, (137) 2018. 10.1007/s00214-018-2235-y

Bukharov, M. S.; Shtyrlin, V. G.; Gilyazetdinov, E. M.; Serov, N. Y.; Madzhidov, T. I.  
Hydration of copper(II) amino acids complexes  
*Journal of Computational Chemistry*, (39): 821-826. 2018. 10.1002/jcc.25154

Bulatova, M.; Melekhova, A. A.; Novikov, A. S.; Ivanov, D. M.; Bokach, N. A.  
Redox reactive (RNC)Cu-II species stabilized in the solid state via halogen bond with I-2  
Zeitschrift Fur Kristallographie-Crystalline Materials, (233): 371-377. 2018. 10.1515/zkri-2017-2107

Burianova, V. K.; Bolotin, D. S.; Mikherdov, A. S.; Novikov, A. S.; Mokolokolo, P. P.; Roodt, A.; Boyarskiy, V. P.; Dar'in, D.; Krasavin, M.; Suslonov, V. V.; Zhdanov, A. P.; Zhizhin, K. Y.; Kuznetsov, N. T.

Mechanism of generation of closo-decaborato amidrazones. Intramolecular non-covalent B-H center dot center dot center dot pi(Ph) interaction determines stabilization of the configuration around the amidrazone C=N bond

New Journal of Chemistry, (42): 8693-8703. 2018. 10.1039/c8nj01018h

Burianova, V. K.; Mikherdov, A. S.; Bolotin, D. S.; Novikov, A. S.; Mokolokolo, P. P.; Roodt, A.; Boyarskiy, V. P.; Suslonov, V. V.; Zhdanov, A. P.; Zhizhin, K. Y.; Kuznetsov, N. T.

Electrophilicity of aliphatic nitrilium closo-decaborate clusters: Hyperconjugation provides an unexpected inverse reactivity order

Journal of Organometallic Chemistry, (870): 97-103. 2018. 10.1016/j.jorgancem.2018.06.017

Burks, D. B.; Davis, S.; Lamb, R. W.; Liu, X.; Rodrigues, R. R.; Liyanage, N. P.; Sun, Y. J.; Webster, C. E.; Delcamp, J. H.; Papish, E. T.

Nickel(II) pincer complexes demonstrate that the remote substituent controls catalytic carbon dioxide reduction

Chemical Communications, (54): 3819-3822. 2018. 10.1039/c7cc09507d

Buschbeck-Alvarado, M. E.; Hernandez-Fernandez, G.; Hernandez-Trujillo, J.; Cortes-Guzman, F.; Cuevas, G.

Charge transfer and electron localization as the origin of the anomeric effect in the OCO segment of dimethoxymethane and spiroketals

Journal of Physical Organic Chemistry, (31) 2018. 10.1002/poc.3793

Buszek, R. J.; Soto, D.; Dailey, J. M.; Bolden, S.; Tall, T. L.; Hudgens, L. M.; Marshall, C. A.; Boatz, J. A.; Drake, G. W.

Structures and Binding Energies of Nitrate Plasticizers DEGDN, TEGDN, and Nitroglycerine Propellants Explosives Pyrotechnics, (43): 115-121. 2018. 10.1002/prep.201700203

Cabral, B. J. C.

Born-Oppenheimer molecular dynamics, hydrogen bond interactions and magnetic properties of liquid hydrogen cyanide

Journal of Molecular Liquids, (272): 778-786. 2018. 10.1016/j.molliq.2018.09.092

Cabrera-Trujillo, J. J.; Fernandez, I.

Understanding the Diels-Alder reactivity of 1,2-azaborine analogues  
Tetrahedron, (74): 4289-4294. 2018. 10.1016/j.tet.2018.06.063

Cai, S. L.; Kong, Y. Y.; Xiao, D.; Chen, Y.; Wang, Q. A.

Primary aminomethyl derivatives of kaempferol: hydrogen bond-assisted synthesis, anticancer activity and spectral properties

Organic & Biomolecular Chemistry, (16): 1921-1931. 2018. 10.1039/c7ob02927f

Calbo, J.; Doncel-Gimenez, A.; Arago, J.; Orti, E.

Tuning the optical and electronic properties of perylene diimides through transversal core extension

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2205-4

Cammi, R.; Chen, B.; Rahm, M.

Analytical calculation of pressure for confined atomic and molecular systems using the eXtreme-Pressure Polarizable Continuum Model

Journal of Computational Chemistry, (39): 2243-2250. 2018. 10.1002/jcc.25544

Camps, P.; Lozano, D.; Barbaraci, C.; Font-Bardia, M.; Luque, F. J.; Estarellas, C.

Generation and Reactions of an Octacyclic Hindered Pyramidalized Alkene

Journal of Organic Chemistry, (83): 5420-5430. 2018. 10.1021/acs.joc.8b00212

Cantero-Lopez, P.; Paez-Hernandez, D.; Arratia-Perez, R.

Tuning the molecular antenna effect using donor and acceptor substituents on the optical properties of the (C<sub>5</sub>F<sub>5</sub>)<sub>2</sub>ThMCp<sub>2</sub> (2+) and (C<sub>5</sub>F<sub>5</sub>)<sub>2</sub>ThMCpL<sub>2</sub> (+) complexes, where M = Fe, Ru and Os and L = CO and C<sub>5</sub>H<sub>5</sub>N

New Journal of Chemistry, (42): 11013-11022. 2018. 10.1039/c8nj00179k

Capozzi, M. A. M.; Punzi, A.; Babudri, F.; Musio, R.; Farinola, G. M.

Synthesis and Computational Study of Semicroconaines and Nonsymmetric Croconaines

Journal of Organic Chemistry, (83): 14396-14405. 2018. 10.1021/acs.joc.8b01930

Carreno, A.; Rodriguez, L.; Paez-Hernandez, D.; Martin-Trasanco, R.; Zuniga, C.; Oyarzun, D. P.; Gacitua, M.; Schott, E.; Arratia-Perez, R.; Fuentes, J. A.

Two New Fluorinated Phenol Derivatives Pyridine Schiff Bases: Synthesis, Spectral, Theoretical Characterization, Inclusion in Epichlorohydrin-beta-Cyclodextrin Polymer, and Antifungal Effect

Frontiers in Chemistry, (6) 2018. 10.3389/fchem.2018.00312

Carreno, A.; Zuniga, C.; Paez-Hernandez, D.; Gacitua, M.; Polanco, R.; Otero, C.; Arratia-Perez, R.; Fuentes, J. A.

Study of the structure-bioactivity relationship of three new pyridine Schiff bases: synthesis, spectral characterization, DFT calculations and biological assays

New Journal of Chemistry, (42): 8851-8863. 2018. 10.1039/c8nj00390d

Carrillo-Campos, J.; Riveros-Rosas, H.; Rodriguez-Satres, R.; Munoz-Clares, R. A.

Bona fide choline monooxygenases evolved in Amaranthaceae plants from oxygenases of unknown function: Evidence from phylogenetics, homology modeling and docking studies

Carvalho, F. S.; Braga, J. P.

DFT Study of Small Gold Clusters, Au-n (2 <= n <= 6): Stability and Charge Distribution Using M08-SO Functional

Brazilian Journal of Physics, (48): 390-397. 2018. 10.1007/s13538-018-0577-5

Casals-Sainz, J. L.; Jimenez-Gravalos, F.; Costales, A.; Francisco, E.; Pendas, A. M.

Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools

Journal of Physical Chemistry A, (122): 849-858. 2018. 10.1021/acs.jpca.7b10714

Castellano, M.; Barros, W. P.; Ferrando-Soria, J.; Julve, M.; Lloret, F.; Pasan, J.; Ruiz-Perez, C.; Canadillas-Delgado, L.; Ruiz-Garcia, R.; Cano, J.

Dicopper(II) metallacyclophanes with photoswitchable oligoacene spacers: a joint experimental and computational study on molecular magnetic photoswitches

Journal of Coordination Chemistry, (71): 675-692. 2018. 10.1080/00958972.2018.1433827

Castillo, M. V.; Iramain, M. A.; Davies, L.; Manzur, M. E.; Brandan, S. A.

Evaluation of the structural properties of powerful pesticide dieldrin in different media and their complete vibrational assignment

Journal of Molecular Structure, (1154): 392-405. 2018. 10.1016/j.molstruc.2017.10.065

Castro, L.; Maron, L.

(C5Me5)(2)Y(mu-H)(mu-CH2C5Me4)Y(C5Me5) as a reservoir of electrons for the reduction of PhSSPh and CO2: A theoretical study

Journal of Organometallic Chemistry, (857): 80-87. 2018. 10.1016/j.jorgancem.2017.09.033

Celaya, C. A.; Reina, M.; Muniz, J.; Sansores, L. E.

Are Small Quasi-Fullerenes Capable of Encapsulating Trimetallic Nitrides A(3-x)B(x)N (A, B =Sc, Y, La, x=0-3)? A DFT Study

Chemistryselect, (3): 6791-6801. 2018. 10.1002/slct.201801038

Celik, S.; Kecel-Gunduz, S.; Akyuz, S.; Ozel, A. E.

Structural analysis, spectroscopic characterization and molecular docking studies of the cyclic heptapeptide

Journal of Biomolecular Structure & Dynamics, (36): 2407-2423. 2018.

10.1080/07391102.2017.1356240

Chakraborty, D.; Chattaraj, P. K.

Confinement induced thermodynamic and kinetic facilitation of some Diels-Alder reactions inside a CB 7 cavitand

Journal of Computational Chemistry, (39): 151-160. 2018. 10.1002/jcc.25094

Chandler, G. S.; Sasse, W. H. F.

Bromination of Acridine  
Australian Journal of Chemistry, (71): 285-288. 2018. 10.1071/ch17619

Chang, C. K.; Chen, W. L.; Wu, D. T.; Lin, S. T.  
Improved Directional Hydrogen Bonding Interactions for the Prediction of Activity Coefficients  
with COSMO-SAC  
Industrial & Engineering Chemistry Research, (57): 11229-11238. 2018.  
10.1021/acs.iecr.8b02493

Charlton, R. J.; Fogarty, R. M.; Bogatko, S.; Zuehlsdorff, T. J.; Hine, N. D. M.; Heeney, M.; Horsfield, A. P.;  
Haynes, P. D.  
Implicit and explicit host effects on excitons in pentacene derivatives  
Journal of Chemical Physics, (148) 2018. 10.1063/1.5017285

Chatfield, D. C.; Morozov, A. N.  
Proximal Pocket Controls Alkene Oxidation Selectivity of Cytochrome P450 and  
Chloroperoxidase toward Small, Nonpolar Substrates  
Journal of Physical Chemistry B, (122): 7828-7838. 2018. 10.1021/acs.jpcb.8b04279

Chatterjee, K.; Dopfer, O.  
Infrared Signatures of Protonated Benzonitrile  
Astrophysical Journal, (865) 2018. 10.3847/1538-4357/aad462

Chatterjee, K.; Dopfer, O.  
Microhydration of PAH(+) cations: evolution of hydration network in naphthalene(+)-(H<sub>2</sub>O)(n)  
clusters (n <= 5)  
Chemical Science, (9): 2301-2318. 2018. 10.1039/c7sc05124g

Chatterjee, K.; Dopfer, O.  
Switching of binding site from nonpolar to polar ligands toward cationic benzonitrile revealed by  
infrared spectroscopy  
Journal of Chemical Physics, (149) 2018. 10.1063/1.5057430

Chemes, D. M.; Cutin, E. H.; Alvarez, R. M. S.; Robles, N. L.; Oberhammer, H.  
On the search of the influence of substituents in the structural and vibrational properties of p-  
substituted sulfinylanilines: Study of p-trifluoromethylsulfinylaniline  
Journal of Fluorine Chemistry, (210): 94-101. 2018. 10.1016/j.jfluchem.2018.02.013

Chen, C.; Ma, Y.; Zheng, D. N.; Zhang, J. S.; Ren, T. G.; Wang, L.; Zhang, J. L.  
Influence of different substitution in pyrazolium ionic liquids on catalytic activity for the fixation  
of CO<sub>2</sub> under solvent- and metal-free conditions  
Tetrahedron, (74): 1776-1784. 2018. 10.1016/j.tet.2018.02.027

Chen, C. Y.; Sun, W. M.; Weng, Q. H.; Huang, S.; Kang, J.

Synthesis, Characterization, Optical Property and Bioactivity of the Eu(III) Complex with Aromatic Carboxylic Triazole

Chinese Journal of Structural Chemistry, (37): 1711-1717. 2018. 10.14102/j.cnki.0254-5861.2011-2004

Chen, H. Y.; Liao, P. L.; Mendonca, M. L.; Snurr, R. Q.

Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metal-Organic Framework NU-1000

Journal of Physical Chemistry C, (122): 12362-12368. 2018. 10.1021/acs.jpcc.8b03641

Chen, Q.; Lai, W.

A Computational Study on P2-Type Na-x Ni<sub>1/3</sub>Ti<sub>2/3</sub>O<sub>2</sub> as Bi-Functional Electrode Material for Na-Ion Batteries

Journal of the Electrochemical Society, (165): A3586-A3594. 2018. 10.1149/2.1281814jes

Chen, X.; Chen, Y. X.; Bai, M.; Wang, C. M.; Qi, D. D.; Liu, Q. Y.; Xu, M. X.; Jiang, J. Z.

Distribution of the unpaired electron in neutral bis(phthalocyaninato) yttrium double-deckers: An experimental and theoretical combinative investigation

Journal of Porphyrins and Phthalocyanines, (22): 165-172. 2018. 10.1142/s1088424618500219

Chen, X.; Wang, C. M.; Chen, Y. X.; Qi, D. D.; Jiang, J. Z.

Vibrational spectra of alkylamino substituted phthalocyanine compounds: Density functional theory calculations

Journal of Porphyrins and Phthalocyanines, (22): 771-776. 2018. 10.1142/s1088424618500591

Chen, X. T.; Li, Q. N.; Gong, Y.

Formation and Characterization of Zr<sup>4+</sup> Stabilized by Neutral Tridentate Ligands in the Gas Phase

Journal of the American Society for Mass Spectrometry, (29): 2327-2332. 2018. 10.1007/s13361-018-2057-0

Chen, X. T.; Li, Q. N. A.; Andrews, L.; Gong, Y.

Infrared Spectroscopic and Theoretical Studies of Group 3 Metal Isocyanide Molecules

Journal of Physical Chemistry A, (122): 7099-7106. 2018. 10.1021/acs.jpca.8b06810

Chen, Z.; Chen, H. W.; Hou, D.; Ren, Y. J.; Zhu, H. M.; Li, L.

Theoretical study on the isomerization process of retinal in gas and aqueous phase

Computational and Theoretical Chemistry, (1146): 15-20. 2018. 10.1016/j.comptc.2018.11.003

Cheng, X. L.; Li, Y. F.; Zhao, Y. Y.; Liu, Y. J.

Reaction Mechanism of Rh (I)-catalyzed Olefin Carboacylation: Enantioselectivity in the Formation of Chiral Poly-fused Rings

Chemical Journal of Chinese Universities-Chinese, (39): 521-529. 2018. 10.7503/cjcu20170405

Cheng, Z. W.; Yang, B. W.; Chen, Q. C.; Ji, W. C.; Shen, Z. M.  
Characteristics and difference of oxidation and coagulation mechanisms for the removal of organic compounds by quantum parameter analysis  
Chemical Engineering Journal, (332): 351-360. 2018. 10.1016/j.cej.2017.09.065

Chermahini, A. N.; Farrokhpour, H.; Shahangi, F.; Dabbagh, H. A.  
Cyclic peptide nanocapsule as ion carrier for halides: a theoretical survey  
Structural Chemistry, (29): 1351-1357. 2018. 10.1007/s11224-018-1117-1

Chioma, F.; Ekennia, A. C.; Ibeji, C. U.; Okafor, S. N.; Onwudiwe, D. C.; Osowole, A. A.; Ujam, O. T.  
Synthesis, characterization, antimicrobial activity and DFT studies of 2-(pyrimidin-2-ylamino)naphthalene-1,4-dione and its Mn(II), Co(II), Ni(II) and Zn(II) complexes  
Journal of Molecular Structure, (1163): 455-464. 2018. 10.1016/j.molstruc.2018.03.025

Chioma, F.; Ekennia, A. C.; Osowole, A. A.; Okafor, S. N.; Ibeji, C. U.; Onwudiwe, D. C.; Ujam, O. T.  
Synthesis, characterization, in-vitro antimicrobial properties, molecular docking and DFT studies of 3-{(E)- (4,6-dimethylpyrimidin-2-yl)imino methyl}naphthalen-2-oland Heteroleptic Mn(II), Co(II), Ni(II) and Zn(II) complexes  
Open Chemistry, (16): 184-200. 2018. 10.1515/chem-2018-0020

Chipman, A.; Gouranourimi, A.; Farshadfar, K.; Olding, A.; Yates, B. F.; Ariafard, A.  
A Computational Mechanistic Investigation into Reduction of Gold(III) Complexes by Amino Acid Glycine: A New Variant for Amine Oxidation  
Chemistry-a European Journal, (24): 8361-8368. 2018. 10.1002/chem.201800403

Chitsazi, R.; Veals, J. D.; Shi, Y.; Sewell, T.  
Correlated Molecular Orbital Theory Study of the Al + CO<sub>2</sub> Reaction  
Journal of Physical Chemistry A, (122): 859-868. 2018. 10.1021/acs.jpca.7b11443

Cho, H. G.; Andrews, L.  
Matrix Infrared Spectroscopic and Theoretical Studies for the Products of Lead Atom Reactions with Ethane and Halomethanes  
Journal of Physical Chemistry A, (122): 8911-8922. 2018. 10.1021/acs.jpca.8b08505

Choi, E.; Lee, C. H.; Jun, B.; Nam, E. B.; Jeong, H.; Lee, S. U.  
Efficiency Tuning of UVA/UVB Absorbance through Control over the Intramolecular Hydrogen Bonding of Triazine Derivatives  
Bulletin of the Korean Chemical Society, (39): 858-863. 2018. 10.1002/bkcs.11487

Chopra, G.; Chopra, N.; Kaur, D.  
Quantum chemical study of hydrogen-bonded complexes of serine with water and H<sub>2</sub>O<sub>2</sub>  
Journal of Chemical Sciences, (130) 2018. 10.1007/s12039-018-1506-4

Chopra, G.; Kaur, D.; Chopra, N.

Modeling protein-protein interactions through alanine-amide hydrogen bonds  
Structural Chemistry, (29): 1397-1415. 2018. 10.1007/s11224-018-1127-z

Chopra, N.; Kaur, D.; Chopra, G.

Hydrogen bonded complexes of oxazole family: electronic structure, stability, and reactivity aspects  
Structural Chemistry, (29): 341-357. 2018. 10.1007/s11224-017-1032-x

Chopra, N.; Kaur, D.; Chopra, G.

Nature and Hierarchy of Hydrogen-Bonding Interactions in Binary Complexes of Azoles with Water and Hydrogen Peroxide  
ACS Omega, (3): 12688-12702. 2018. 10.1021/acsomega.8b01523

Chopra, P.; Chakraborty, S.

Computational study of red-and blue-shifted C-H center dot center dot center dot Se hydrogen bond in Q(3)C-H center dot center dot center dot SeH<sub>2</sub> ( Q = Cl, F, H) complexes  
Chemical Physics, (500): 54-61. 2018. 10.1016/j.chemphys.2017.11.010

Choubane, H.; Garrido-Castro, A. F.; Alvarado, C.; Martin-Somer, A.; Guerrero-Corella, A.; Daaou, M.; Diaz-Tendero, S.; Maestro, M. C.; Fraile, A.; Aleman, J.

Intramolecular hydrogen-bond activation for the addition of nucleophilic imines: 2-hydroxybenzophenone as a chemical auxiliary  
Chemical Communications, (54): 3399-3402. 2018. 10.1039/c8cc01479e

Choudhuri, K.; Pramanik, M.; Mandal, A.; Mal, P.

S-H center dot center dot center dot pi Driven Anti-Markovnikov Thiol-Yne Click Reaction  
Asian Journal of Organic Chemistry, (7): 1849-1855. 2018. 10.1002/ajoc.201800381

Chowdhury, M. G.; Barik, S. K.; Saha, K.; Kirubakaran, B.; Banerjee, A.; Ramkumar, V.; Ghosh, S.  
Electron Precise Group 5 Dimetalla heteroboranes {CpV(mu-EPh)}<sub>2</sub>{mu-eta(2):eta(2)-BH<sub>3</sub>E} and {CpNb((mu-EPh)}<sub>2</sub>{mu-eta(2):eta(2)-B<sub>2</sub>H<sub>4</sub>E} (E = S or Se)  
Inorganic Chemistry, (57): 985-994. 2018. 10.1021/acs.inorgchem.7b02305

Chrostowska, A.; Darrigan, C.; Dargelos, A.; Graciaa, A.; Guillemin, J. C.

Isoselenocyanates versus Isothiocyanates and Isocyanates  
Journal of Physical Chemistry A, (122): 2894-2905. 2018. 10.1021/acs.jpca.7b12604

Ciancaleoni, G.

Cooperativity between hydrogen- and halogen bonds: the case of selenourea  
Physical Chemistry Chemical Physics, (20): 8506-8514. 2018. 10.1039/c8cp00353j

Ciancaleoni, G.

Lewis Base Activation of Lewis Acid: A Detailed Bond Analysis  
ACS Omega, (3): 16292-16300. 2018. 10.1021/acsomega.8b02243

Cicac-Hudi, M.; Schlindwein, S. H.; Feil, C. M.; Nieger, M.; Gudat, D.  
Cationic Diiodo-Phosphoranides through Oxidative I-2 Addition to Tricyclic Phosphamethine  
Cyanines  
Zeitschrift fur Anorganische und Allgemeine Chemie, (644): 1304-1310. 2018.  
10.1002/zaac.201800264

Cicac-Hudi, M.; Schlindwein, S. H.; Feil, C. M.; Nieger, M.; Gudat, D.  
Isolable N-heterocyclic carbene adducts of the elusive diiodophosphine  
Chemical Communications, (54): 7645-7648. 2018. 10.1039/c8cc03972k

Cisneros, G. I. V.; Vasquez-Perez, J. M.; Cruz-Borbolla, J.; Gomez-Castro, C. Z.; Nicolas-Vazquez, M. I.;  
Ruvalcaba, R. M.  
Theoretical study: Electronic structure and receptor interaction of four type bis-1,4-dihdropyridine molecules  
Computational and Theoretical Chemistry, (1123): 102-110. 2018.  
10.1016/j.comptc.2017.11.012

Clark, T.; Hesselmann, A.  
The coulombic sigma-hole model describes bonding in CX3I center dot center dot center dot Y-complexes completely  
Physical Chemistry Chemical Physics, (20): 22849-22855. 2018. 10.1039/c8cp03079k

Clark, T.; Murray, J. S.; Politzer, P.  
A perspective on quantum mechanics and chemical concepts in describing noncovalent interactions  
Physical Chemistry Chemical Physics, (20): 30076-30082. 2018. 10.1039/c8cp06786d

Coa, J. C.; Cardona-Galeano, W.; Restrepo, A.  
Fe<sup>3+</sup> chelating quinoline-hydrazone hybrids with proven cytotoxicity, leishmanicidal, and trypanocidal activities  
Physical Chemistry Chemical Physics, (20): 20382-20390. 2018. 10.1039/c8cp04174a

Coburger, P.; Aures, R.; Schulz, P.; Hey-Hawkins, E.  
Exploiting the Ring Strain of Diphosphetanes: A Synthetic and Computational Approach towards 1,2,5-Selenadiphospholanes  
Chempluschem, (83): 1057-1064. 2018. 10.1002/cplu.201800391

Cortes-Arriagada, D.; Villegas-Escobar, N.; Ortega, D. E.  
Fe-doped graphene nanosheet as an adsorption platform of harmful gas molecules (CO, CO<sub>2</sub>, SO<sub>2</sub> and H<sub>2</sub>S), and the co-adsorption in O<sub>2</sub> environments  
Applied Surface Science, (427): 227-236. 2018. 10.1016/j.apsusc.2017.08.216

Costa, A.; Costa, E. R.; Silva, A. L. P.; Tanaka, A. A.; Varela, J. D. G.

Theoretical study of the effects of substituents (F, Cl, Br, CH<sub>3</sub>, and CN) on the aromaticity of borazine

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-017-3555-x

Costa, M. P. M.; Prates, L. M.; Baptista, L.; Cruz, M. T. M.; Ferreira, I. L. M.

Interaction of polyelectrolyte complex between sodium alginate and chitosan dimers with a single glyphosate molecule: A DFT and NBO study

Carbohydrate Polymers, (198): 51-60. 2018. 10.1016/j.carbpol.2018.06.052

Costa, R. A.; Junior, E. S. A.; Lopes, G. B. P.; Pinheiro, M. L. B.; Costa, E. V.; Bezerra, D. P.; Oliveira, K.

Structural, vibrational, UV-vis, quantum-chemical properties, molecular docking and anti-cancer activity study of annomantine and N-hydroxyannomantine beta-carboline alkaloids: A combined experimental and DFT approach

Journal of Molecular Structure, (1171): 682-695. 2018. 10.1016/j.molstruc.2018.06.054

Costa, R. A.; Oliveira, K. M. T.; Nunomura, R. D. S.; Junior, E. S. A.; Pinheiro, M. L. B.; Costa, E. V.; Barison, A.

Quantum chemical properties investigation and molecular docking analysis with DNA topoisomerase II of beta-carboline indole alkaloids from Simaba guianensis: a combined experimental and theoretical DFT study

Structural Chemistry, (29): 299-314. 2018. 10.1007/s11224-017-1029-5

Crawford, J. M.; Stone, E. A.; Metrano, A. J.; Miller, S. J.; Sigman, M. S.

Parameterization and Analysis of Peptide-Based Catalysts for the Atroposelective Bromination of 3-Arylquinazolin-4(3H)-ones

Journal of the American Chemical Society, (140): 868-871. 2018. 10.1021/jacs.7b11303

Cruz, F.; Vaz, B.; Vilar, U.; Ortega, A.; Madich, Y.; Alvarez, R.; Aurrecochea, J. M.

Regioselective Palladium-Catalyzed Heterocyclization-Sonogashira Coupling Cascades from 2-Alkynylbenzamides and Terminal Alkynes: Experimental and DFT Studies

Organometallics, (37): 3813-3826. 2018. 10.1021/acs.organomet.8b00519

Cuerva, C.; Morais, N.; Campo, J. A.; Cano, M.; Lodeiro, C.

Isoquinolinylpyrazoles and pyridylisoxazoles as luminescent materials with sensorial ability towards pollutant toxic metal ions. Experimental and computational studies

Journal of Luminescence, (198): 517-530. 2018. 10.1016/j.jlumin.2018.02.058

Cui, G. K.; Li, Y. N.; Liu, J. X.; Wang, H. Y.; Li, Z. Y.; Wang, J. J.

Tuning Environmentally Friendly Chelate-Based Ionic Liquids for Highly Efficient and Reversible SO<sub>2</sub> Chemisorption

ACS Sustainable Chemistry & Engineering, (6): 15292-15300. 2018.

10.1021/acssuschemeng.8b03748

Cui, Y. Q.; Cui, X. H.; Zhang, L.; Xie, Y. J.; Yang, M. L.

Theoretical characterization on the size-dependent electron and hole trapping activity of chloride-passivated CdSe nanoclusters

Journal of Chemical Physics, (148) 2018. 10.1063/1.5023408

Cui, Z. H.; Aquino, A. J. A.; Sue, A. C. H.; Lischka, H.

Analysis of charge transfer transitions in stacked pi-electron donor-acceptor complexes

Physical Chemistry Chemical Physics, (20): 26957-26967. 2018. 10.1039/c8cp04770g

Curran, D.; Dada, O.; Muller-Bunz, H.; Rothemund, M.; Sanchez-Sanz, G.; Schobert, R.; Zhu, X. M.; Tacke, M.

Synthesis and Cytotoxicity Studies of Novel NHC\*-Gold(I) Complexes Derived from Lepidiline A Molecules, (23) 2018. 10.3390/molecules23082031

da Silva, A. R. L.; dos Santosa, A. J.; Martinez-Huitle, C. A.

Electrochemical measurements and theoretical studies for understanding the behavior of catechol, resorcinol and hydroquinone on the boron doped diamond surface

RSC Advances, (8): 3483-3492. 2018. 10.1039/c7ra12257h

da Silva, V. H. M.; Quattrociocchi, D. G. S.; Stoyanov, S. R.; Carneiro, J. W. D.; da Costa, L. M.; Ferreira, G. B.

A DFT study of the interaction between Cd(H<sub>2</sub>O)(3) (2+) and monodentate O-, N-, and S-donor ligands: bond interaction analysis

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-017-3571-x

Dahanayake, J. N.; Kasireddy, C.; Karnes, J. P.; Verma, R.; Steinert, R. M.; Hildebrandt, D.; Hull, O. A.; Ellis, J. M.; Mitchell-Koch, K. R.

Progress in Our Understanding of F-19 Chemical Shifts

Annual Reports on Nmr Spectroscopy, Vol 93, (93): 281-365. 2018.

10.1016/bs.arnmr.2017.08.002

Dahlkamp, J. M.; Tolzmann, M.; Lucchesi, R.; Daniliuc, C. G.; Wibbeling, B.; Uhl, W.; Wurthwein, E. U.

Chemoselective Hydroalumination of 1-Aza-but-1-en-3-yne (C-Iminoalkynes): Formation of Propargylamines by Imine Reduction and of 5-Aluminazoles and 1-Aza-butadienes by Anti-Michael Attack

Organometallics, (37): 1346-1357. 2018. 10.1021/acs.organomet.8b00036

Dahmani, R.; Ben Yaghlane, S.; Boughdiri, S.; Al-Mogren, M. M.; Prakash, M.; Hochlaf, M.

Insights on the interaction of Zn<sup>2+</sup> cation with triazoles: Structures, bonding, electronic excitation and applications

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (193): 375-384. 2018.

10.1016/j.saa.2017.12.017

Dai, G. L.; Chen, L.; Xie, F. M.

Structures and electronic properties of halogenated Au(III) phthalocyanine AuPcX (X = Cl, Br): A Density Functional Theoretical Study

Computational Materials Science, (152): 262-267. 2018. 10.1016/j.commatsci.2018.06.007

Dai, G. L.; Chen, L.; Zhao, X.

Tungsten-Embedded Graphene: Theoretical Study on a Potential High-Activity Catalyst toward CO Oxidation

Materials, (11) 2018. 10.3390/ma11101848

Dai, W. S.; Liu, S.; Zhang, Z.; Chi, X. P.; Cheng, M.; Du, Y. K.; Zhu, Q. H.

Conformational preferences and isomerization upon excitation/ionization of 2-methoxypyridine and 2-N-methylaminopyridine

Physical Chemistry Chemical Physics, (20): 6211-6226. 2018. 10.1039/c7cp07854d

Dajnowicz, S.; Parks, J. M.; Hu, X. C.; Johnston, R. C.; Kovalevsky, A. Y.; Mueser, T. C.

Hyperconjugation Promotes Catalysis in a Pyridoxal 5'-Phosphate-Dependent Enzyme

ACS Catalysis

(8): 6733-6737. 2018. 10.1021/acscatal.8b01911

Dakkouri, M.; Girichev, G.; Giricheva, N.; Petrov, V.; Petrova, V.

Structural analysis and probing the conformational space of dansylamide by means of gas-phase electron diffraction and quantum chemistry

Structural Chemistry, (29): 823-835. 2018. 10.1007/s11224-018-1108-2

Dang, Y. R.; Meng, L. P.; Qin, M.; Li, Q. Z.; Li, X. Y.

Stability and donor-acceptor bond in dinuclear organometallics CpM1-M2Cl3 (M-1, M-2 = B, Al, Ga, In; Cp = eta(5)-C5H5)

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-017-3539-x

Dang, Y. R.; Wang, W. H.; Meng, L. P.; Li, Q. Z.; Li, X. Y.

Nature of MoH center dot center dot center dot I bonds in Cp2Mo(L)H center dot center dot center dot center dot I-CC-R Complexes (L=H, CN, PPh2, C(CH3)(3); R=NO2, Cl, Br, H, OH, CH3, NH2)

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4258

Danrioyi, N. E.; Friedrich, H. B.; Kruger, G. H.; Willock, D.

A DFT mechanistic study of the ODH of n-hexane over isolated H3VO4

Molecular Catalysis, (452): 83-92. 2018. 10.1016/j.mcat.2018.03.019

Das, A. K.; Demerdash, O. N.; Head-Gordon, T.

Improvements to the AMOEBA Force Field by Introducing Anisotropic Atomic Polarizability of the Water Molecule

Journal of Chemical Theory and Computation, (14): 6722-6733. 2018. 10.1021/acs.jctc.8b00978

Daswani, U.; Singh, U.; Sharma, P.; Kumar, A.

From Molecules to Devices: A DFT/TD-DFT Study of Dipole Moment and Internal Reorganization Energies in Optoelectronically Active Aryl Azo Chromophores

Journal of Physical Chemistry C, (122): 14390-14401. 2018. 10.1021/acs.jpcc.8b04070

Davis-Gilbert, Z. W.; Wen, X. L.; Goodpaster, J. D.; Tonks, I. A.

Mechanism of Ti-Catalyzed Oxidative Nitrene Transfer in 2+2+1 Pyrrole Synthesis from Alkynes and Azobenzene

Journal of the American Chemical Society, (140): 7267-7281. 2018. 10.1021/jacs.8b03546

de Carvalho, E. F. V.; Lopez-Castillo, A.; Roberto-Neto, O.

A comparative study of the structures and electronic properties of graphene fragments: A DFT and MP2 survey

Chemical Physics Letters, (691): 291-297. 2018. 10.1016/j.cplett.2017.11.023

de la Concepcion, J. G.; Avalos, M.; Cintas, P.; Jimenez, J. L.; Light, M. E.

Mechanistic studies of 1,3-dipolar cycloadditions of bicyclic thioisomunchnones with alkenes. A computational rationale focused on donor-acceptor interactions

Organic & Biomolecular Chemistry, (16): 3438-3452. 2018. 10.1039/c8ob00683k

de la Luz, A. P.; Aguilar-Pineda, J. A.; Mendez-Bermudez, J. G.; Alejandre, J.

Force Field Parametrization from the Hirshfeld Molecular Electronic Density

Journal of Chemical Theory and Computation, (14): 5949-5958. 2018. 10.1021/acs.jctc.8b00554

de Lange, J. H.; Cukrowski, I.

Exact and exclusive electron localization indices within QTAIM atomic basins

Journal of Computational Chemistry, (39): 1517-1530. 2018. 10.1002/jcc.25223

de Melo, U. Z.; Yamazaki, D. A. D.; Candido, A. D.; Basso, E. A.; Gauze, G. D.

DFT calculations and NMR measurements applied to the conformational analysis of cis and trans-3-phenylaminocyclohexyl N,N-dimethylcarbamates

Journal of Molecular Structure, (1163): 227-235. 2018. 10.1016/j.molstruc.2018.01.096

de Oliveira, A. Z.; Campos, C. T.; Jorge, F. E.; Ferreira, I. B.; Fantin, P. A.

All-electron triple zeta basis sets for the actinides

Computational and Theoretical Chemistry, (1135): 28-33. 2018. 10.1016/j.comptc.2018.05.010

de Rezende, F. M. P.; Freitas, M. P.; Ramalho, T. C.

Probing long-range spin-spin coupling constants in 2-halo-substituted cyclohexanones and cyclohexanethiones: The role of solvent and stereoelectronic effects

Magnetic Resonance in Chemistry, (56): 810-816. 2018. 10.1002/mrc.4739

De, S.; Rinsha, C. H.; Thamleena, A. H.; Joseph, A.; Ben, A.; Krishnapriya, V. U.

Roles of different amino-acid residues towards binding and selective transport of K<sup>+</sup> through KcsA K<sup>+</sup>-ion channel

Physical Chemistry Chemical Physics, (20): 17517-17529. 2018. 10.1039/c8cp01282b

De Vleeschouwer, F.; Denayer, M.; Pinter, B.; Geerlings, P.; De Proft, F.

Characterization of chalcogen bonding interactions via an in-depth conceptual quantum chemical analysis

Journal of Computational Chemistry, (39): 557-572. 2018. 10.1002/jcc.25099

De Vlugt, I. J. S.; Lecours, M. J.; Carr, P. J. J.; Anwar, A.; Marta, R. A.; Fillion, E.; Steinmetz, V.; Hopkins, W. S.

Infrared-Driven Charge-Transfer in Transition Metal-Containing B<sub>12</sub>X<sub>12</sub>- (X = H, F) Clusters

Journal of Physical Chemistry A, (122): 7051-7061. 2018. 10.1021/acs.jpca.8b05750

Deak, N.; Septean, R.; Moraru, I. T.; Mallet-Ladeira, S.; Madec, D.; Nemes, G.

PALLADIUM AND RUTHENIUM DERIVATIVES STABILISED BY BIS-SULFONE LIGAND

Studia Universitatis Babes-Bolyai Chemia, (63): 105-115. 2018. 10.24193/subbchem.2018.2.10

Deb, J.; Paul, D.; Sarkar, U.; Ayers, P. W.

Characterizing the sensitivity of bonds to the curvature of carbon nanotubes

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3793-6

Deb, P.; Jin, G. Y.; Singh, S. K.; Moon, J.; Kwon, H.; Das, A.; Bagchi, S.; Kim, Y. S.

Interconverting Hydrogen-Bonding and Weak n → π\* Interactions in Aqueous Solution: A Direct Spectroscopic Evidence

Journal of Physical Chemistry Letters, (9): 5425-5429. 2018. 10.1021/acs.jpclett.8b02398

DeBackere, J. R.; Schrobilgen, G. J.

A Homoleptic KrF<sub>2</sub> Complex, Hg(KrF<sub>2</sub>)<sub>(8)</sub> AsF<sub>6</sub> (2)center dot 2HF

Angewandte Chemie-International Edition, (57): 13167-13171. 2018. 10.1002/anie.201807755

Dede, B.; Avci, D.; Bahceli, S.

Study on the 4-ethoxy-2-methyl-5-(4-morpholinyl)-3(2H)pyridazinone using FT-IR, H-1 and C-13 NMR, UV-vis spectroscopy, and DFT/HSEH1PBE method

Canadian Journal of Physics, (96): 1042-1052. 2018. 10.1139/cjp-2017-0508

Dede, B.; Avci, D.; Varkal, D.; Bahceli, S.

Molecular, Spectroscopic, NBO and NLO Properties of 4-Methyl-5-thiazoleethanol: A Comparative Theoretical Study

Acta Physica Polonica A, (134): 1083-1091. 2018. 10.12693/APhysPolA.134.1083

Deepa, P.; Pandiyan, B. V.; Kolandaivel, P.

Does the presence of water clusters induce the binding affinity of CK2 halogen ligands?: A quantum chemical perspective study

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25644

Deilami, A. B.; Salehi, M.; Arab, A.; Amiri, A.  
Synthesis, crystal structure, electrochemical properties and DFT calculations of three new Zn(II), Ni(II) and Co(III) complexes based on 5-bromo-2-((allylimino)methyl) phenol Schiff-based ligand  
*Inorganica Chimica Acta*, (476): 93-100. 2018. 10.1016/j.ica.2018.02.013

Del Bene, J. E.; Alkorta, I.; Elguero, J.  
Hydrogen and Halogen Bonding in Cyclic FH(4-n):FCI,Complexes, for n=0-4  
*Journal of Physical Chemistry A*, (122): 2587-2597. 2018. 10.1021/acs.jpca.8b00236

Del Bene, J. E.; Alkorta, I.; Montero-Campillo, M. M.; Elguero, J.  
Using protonation to change a Cl center dot center dot center dot N halogen bond in N-Base:  
ClOH complexes to a Cl center dot center dot center dot O halogen bond  
*Chemical Physics Letters*, (710): 123-128. 2018. 10.1016/j.cplett.2018.08.027

Del Bene, J. E.; Elguero, J.; Alkorta, I.  
Complexes of CO<sub>2</sub> with the Azoles: Tetrel Bonds, Hydrogen Bonds and Other Secondary  
Interactions  
*Molecules*, (23) 2018. 10.3390/molecules23040906

Demerdash, O.; Wang, L. P.; Head-Gordon, T.  
Advanced models for water simulations  
*Wiley Interdisciplinary Reviews-Computational Molecular Science*, (8) 2018. 10.1002/wcms.1355

Demircioglu, Z.; Kastas, C. A.; Buyukgungor, O.  
XRD, Ff-IR and UV characterization, hirshfeld surface analysis and local-global chemical  
descriptor studies of (E)-2-((3-fluorophenylimino)methyl)-3-methoxyphenol (1) and (E)-2-((2-  
fluorophenylimino)methyl)-3-methoxyphenol (2)  
*Journal of Molecular Structure*, (1166): 131-146. 2018. 10.1016/j.molstruc.2018.04.030

Demircioglu, Z.; Ozdemir, F. A.; Dayan, O.; Serbetci, Z.; Ozdemir, N.  
Synthesis, X-ray diffraction method, spectroscopic characterization (FT-IR, H-1 and C-13 NMR),  
antimicrobial activity, Hirshfeld surface analysis and DFT computations of novel sulfonamide derivatives  
*Journal of Molecular Structure*, (1161): 122-137. 2018. 10.1016/j.molstruc.2018.02.063

Demircioglu, Z.; Yesil, A. E.; Altun, M.; Bal-Demirci, T.; Ozdemir, N.  
X-ray structure determination, Hirshfeld surface analysis, spectroscopic (FT-IR, NMR, UV-Vis,  
fluorescence), non-linear optical properties, Fukui function and chemical activity of 4 '(2,4-  
dimethoxyphenyl)-2,2 ':6 ',2 "-terpyridine  
*Journal of Molecular Structure*, (1162): 96-108. 2018. 10.1016/j.molstruc.2018.02.093

Denavit, V.; Laine, D.; St-Gelais, J.; Johnson, P. A.; Giguere, D.  
A Chiron approach towards the stereoselective synthesis of polyfluorinated carbohydrates  
*Nature Communications*, (9) 2018. 10.1038/s41467-018-06901-y

Denny, M. S.; Parent, L. R.; Patterson, J. P.; Meena, S. K.; Pham, H.; Abellan, P.; Ramasse, Q. M.; Paesani, F.; Gianneschi, N. C.; Cohen, S. M.

Transmission Electron Microscopy Reveals Deposition of Metal Oxide Coatings onto Metal-Organic Frameworks

Journal of the American Chemical Society, (140): 1348-1357. 2018. 10.1021/jacs.7b10453

Devi, P.; Fatma, S.; Bishnoi, A.; Srivastava, K.; Shukla, S.; Kumar, R.

Synthesis, spectroscopic and DFT studies of novel 4-(morpholinomethyl)-5-oxo-1-phenylpyrrolidine-3-carboxylic acid

Journal of Molecular Structure, (1157): 551-559. 2018. 10.1016/j.molstruc.2017.12.065

Devi, P.; Fatma, S.; Parveen, H.; Bishnoi, A.; Singh, R.

Spectroscopic analysis, first order hyperpolarizability, NBO, HOMO and LUMO analysis of 5-oxo-1-phenylpyrrolidine-3-carboxylic acid: Experimental and theoretical approach

Indian Journal of Pure & Applied Physics, (56): 814-829. 2018.

Devi, S.; Saraswat, M.; Grewal, S.; Venkataramani, S.

Evaluation of Substituent Effect in Z-Isomer Stability of Arylazo-1H-3,5-dimethylpyrazoles: Interplay of Steric, Electronic Effects and Hydrogen Bonding

Journal of Organic Chemistry, (83): 4307-4322. 2018. 10.1021/acs.joc.7b02604

Dhanishta, P.; Kumar, P. S. S.; Mishra, S. K.; Suryaprakash, N.

Intramolecular hydrogen bond directed stable conformations of benzoyl phenyl oxalamides: unambiguous evidence from extensive NMR studies and DFT-based computations

RSC Advances, (8): 11230-11240. 2018. 10.1039/c8ra00357b

Dhanishta, P.; Mishra, S. K.; Suryaprakash, N.

Intramolecular HB Interactions Evidenced in Dibenzoyl Oxalamide Derivatives: NMR, QTAIM, and NCI Studies

Journal of Physical Chemistry A, (122): 199-208. 2018. 10.1021/acs.jpca.7b10598

Dharmawardhana, C. C.; Misra, A.; Ching, W. Y.

Theoretical investigation of C-(A)-S-H(I) cement hydrates

Construction and Building Materials, (184): 536-548. 2018. 10.1016/j.conbuildmat.2018.07.004

Dheivamalar, S.; Sugi, L.; Ravichandran, K.; Sriram, S.

Adsorption of alanine with heteroatom substituted fullerene for solar cell application: A DFT study

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (202): 333-345. 2018. 10.1016/j.saa.2018.05.039

Diaz-Cervantes, E.; Robles, J.; Aguilera-Granja, F.

Understanding the structure, electronic properties, solubility in water, and protein interactions of three novel nano-devices against ovarian cancer: a computational study

Journal of Nanoparticle Research, (20) 2018. 10.1007/s11051-018-4362-8

Dietrich, C.; Koerver, R.; Gaultois, M. W.; Kieslich, G.; Cibin, G.; Janek, J.; Zeier, W. G.

Spectroscopic characterization of lithium thiophosphates by XPS and XAS - a model to help monitor interfacial reactions in all-solid-state batteries

Physical Chemistry Chemical Physics, (20): 20088-20095. 2018. 10.1039/c8cp01968a

Dikmen, G.; Alver, O.; Parlak, C.

NMR determination of solvent dependent behavior and XRD structural properties of 4-carboxy phenylboronic acid: A DFT supported study

Chemical Physics Letters, (698): 114-119. 2018. 10.1016/j.cplett.2018.03.005

Dimic, D.

The importance of specific solvent-solute interactions for studying UV-vis spectra of light-responsive molecular switches

Comptes Rendus Chimie, (21): 1001-1010. 2018. 10.1016/j.crci.2018.09.007

Dimic, D.; Milenkovic, D.; Ilic, J.; Smit, B.; Amic, A.; Markovic, Z.; Markovic, J. D.

Experimental and theoretical elucidation of structural and antioxidant properties of vanillylmandelic acid and its carboxylate anion

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (198): 61-70. 2018. 10.1016/j.saa.2018.02.063

Dimic, D. S.; Milenkovic, D. A.; Markovic, J. M. D.; Markovic, Z. S.

Thermodynamic and kinetic analysis of the reaction between biological catecholamines and chlorinated methylperoxy radicals

Molecular Physics, (116): 1166-1178. 2018. 10.1080/00268976.2017.1414967

Ding, W. J.; Liu, Y. X.; Wang, D. Q.

Computational Comparative Mechanistic Study of C-E (E=C,N,O,S) Coupling Reactions through CO<sub>2</sub> Activation Mediated by Uranium(III) Complexes

Chemistry-a European Journal, (24): 19289-19299. 2018. 10.1002/chem.201804072

Ding, X. Q.; Ding, J. J.; Li, D. Y.; Pan, L.; Pei, C. X.

Toxicity Prediction of Organophosphorus Chemical Reactivity Compounds Based on Conceptual DFT

Acta Physico-Chimica Sinica, (34): 314-322. 2018. 10.3866/pku.Whxb201709042

Ding, Y. Q.; Li, J. Y.; Wang, S. J.; Junzhang; Mu, Q. H.; Wang, J. G.

Reactions of aldehyde with collagen: a DFT study

Structural Chemistry, (29): 1499-1510. 2018. 10.1007/s11224-018-1131-3

Diniz, J. R.; de Lima, T. B.; Galaverna, R.; de Oliveira, A. L.; Ferreira, D. A. C.; Gozzo, F. C.; Eberlin, M. N.; Dupont, J.; Neto, B. A. D.

Is the formation of N-heterocyclic carbenes (NHCs) a feasible mechanism for the distillation of imidazolium ionic liquids?

Physical Chemistry Chemical Physics, (20): 24716-24725. 2018. 10.1039/c8cp03609h

Divya, P.; Jothy, V. B.

Density functional theoretical analysis with experimental, invitro bioactivity and molecular docking investigations on the pesticide Albendazole

Chemical Physics Letters, (695): 1-7. 2018. 10.1016/j.cplett.2018.01.055

Divya, P.; Muthuraja, P.; Dhandapani, M.; Jothy, V. B.

Pesticidal compound Pirimicarb: Spectral analysis, DFT computations, molecular docking study and in vitro bioactivity

Chemical Physics Letters, (706): 295-302. 2018. 10.1016/j.cplett.2018.06.021

Doan, H. A.; Li, Z. Y.; Farha, O. K.; Hupp, J. T.; Snurr, R. Q.

Theoretical insights into direct methane to methanol conversion over supported dicopper oxo nanoclusters

Catalysis Today, (312): 2-9. 2018. 10.1016/j.cattod.2018.03.063

Dobrowolski, J. C.; Lipinski, P. F. J.; Karpinska, G.

Substituent Effect in the First Excited Singlet State of Monosubstituted Benzenes

Journal of Physical Chemistry A, (122): 4609-4621. 2018. 10.1021/acs.jpca.8b02209

Dodson, L. G.; Thompson, M. C.; Weber, J. M.

Interactions of Molecular Titanium Oxides TiO<sub>x</sub> (x=1-3) with Carbon Dioxide in Cluster Anions

Journal of Physical Chemistry A, (122): 6909-6917. 2018. 10.1021/acs.jpca.8b06229

Dodson, L. G.; Thompson, M. C.; Weber, J. M.

Titanium Insertion into CO Bonds in Anionic Ti-CO<sub>2</sub> Complexes

Journal of Physical Chemistry A, (122): 2983-2991. 2018. 10.1021/acs.jpca.8b01843

Domingo, L. R.; Rios-Gutierrez, M.; Perez, P.

A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels-Alder and Polar Alder-ene Reactions

Molecules, (23) 2018. 10.3390/molecules23081913

Domingo, L. R.; Rios-Gutierrez, M.; Perez, P.

A Molecular Electron Density Theory Study of the Reactivity and Selectivities in 3+2

Cycloaddition Reactions of C,N-Dialkyl Nitrones with Ethylene Derivatives

Journal of Organic Chemistry, (83): 2182-2197. 2018. 10.1021/acs.joc.7603093

Domingo, L. R.; Rios-Gutierrez, M.; Perez, P.

A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine

Ylides in 3+2 Cycloaddition Reactions

Journal of Organic Chemistry, (83): 10959-10973. 2018. 10.1021/acs.joc.8b01605

Domingo, L. R.; Rios-Gutierrez, M.; Silvi, B.; Perez, P.

The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis

European Journal of Organic Chemistry: 1107-1120. 2018. 10.1002/ejoc.201701350

Dong, W. B.; Li, Q. Z.; Scheiner, S.

Comparative Strengths of Tetrel, Pnicogen, Chalcogen, and Halogen Bonds and Contributing Factors

Molecules, (23) 2018. 10.3390/molecules23071681

Dong, W. B.; Wang, Y. Q.; Yang, X.; Cheng, J. B.; Li, Q. Z.

Dual function of the boron center of  $\text{BH}(\text{CO})(2)/\text{BH}(\text{N}-2)(2)$  in halogen- and triel-bonded complexes with hypervalent halogens

Journal of Molecular Graphics & Modelling, (84): 118-124. 2018. 10.1016/j.jmgm.2018.06.017

Dong, X.; Jalife, S.; Vasquez-Espinal, A.; Ravell, E.; Pan, S.; Cabellos, J. L.; Liang, W. Y.; Cui, Z. H.; Merino, G.

$\text{Li}_2\text{B}_{12}$  and  $\text{Li}_3\text{B}_{12}$ : Prediction of the Smallest Tubular and Cage-like Boron Structures  
Angewandte Chemie-International Edition, (57): 4627-4631. 2018. 10.1002/anie.201800976

Dong, X. L.; Deng, G. H.; Wu, Z.; Xu, J.; Lu, B.; Trabelsi, T.; Francisco, J. S.; Zeng, X. Q.

Spectroscopic Identification of  $\text{H}_2\text{NSO}$  and syn- and anti- $\text{HNSOH}$  Radicals

Angewandte Chemie-International Edition, (57): 7513-7517. 2018. 10.1002/anie.201802738

Dorostei, N.; Mohammadpour, H.

Synthesis, characterization and biological evaluation of a nanorod five-coordinated Sn(IV) complex. Theoretical studies of  $(\text{CH}_3)(2)\text{Sn}(\text{O}_2\text{PPh}_2)(2)$

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4610

Drenchev, N.; Rosnes, M. H.; Dietzel, P. D. C.; Albinati, A.; Hadjiivanov, K.; Georgiev, P. A.

Open Metal Sites in the Metal-Organic Framework CPO-27-Cu: Detection of Regular and Defect Copper Species by CO and NO Probe Molecules

Journal of Physical Chemistry C, (122): 17238-17249. 2018. 10.1021/acs.jpcc.8b04045

Drideh, S.; Zouchoune, B.; Zendaoui, S. M.; Saillard, J. Y.

Electronic structure and structural diversity in indenyl in heterobinuclear transition-metal half-sandwich complexes

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2285-1

Du, J. G.; Sun, X. Y.; Zhang, L.; Zhang, C. Y.; Jiang, G.

Hydrogen storage of Li-4&B-36 cluster

Scientific Reports, (8) 2018. 10.1038/s41598-018-20452-8

Du, P.; Zhao, J. Y.

Density Functional Theory Mechanistic Study of Boron-Catalyzed N-Alkylation of Amines with Formic Acid: Formic Acid Activation by Silylation Reaction

Chemistry-an Asian Journal, (13): 701-709. 2018. 10.1002/asia.201701607

Dudev, T.; Grauffel, C.; Lim, C.

How Pb<sup>2+</sup> Binds and Modulates Properties of Ca<sup>2+</sup>-Signaling Proteins

Inorganic Chemistry, (57): 14798-14809. 2018. 10.1021/acs.inorgchem.8b02548

Dudev, T.; Mazmanian, K.; Lim, C.

Competition between Li<sup>+</sup> and Na<sup>+</sup> in sodium transporters and receptors: Which Na<sup>+</sup>-Binding sites are "therapeutic" Li<sup>+</sup> targets?

Chemical Science, (9): 4093-4103. 2018. 10.1039/c7sc05284g

Durand, R. J.; Achelle, S.; Gauthier, S.; Cabon, N.; Ducamp, M.; Kahlal, S.; Saillard, J. Y.; Barsella, A.; Robin-Le Guen, F.

Incorporation of a ferrocene unit in the pi-conjugated structure of donor-linker-acceptor (D-pi-A) chromophores for nonlinear optics (NLO)

Dyes and Pigments, (155): 68-74. 2018. 10.1016/j.dyepig.2018.03.029

Durgadevi, G.; Arjunan, V.; Thirunarayanan, S.; Marchewka, M. K.; Mohan, S.

Structure, electronic, spectroscopic and reactivity investigations of pharmacologically active compound 1-acetyl-3-indolecarboxaldehyde - An experimental and theoretical approach

Journal of Molecular Structure, (1164): 57-69. 2018. 10.1016/j.molstruc.2018.03.045

Dutta, B.; Bhattacharjee, B.; Chowdhury, J.

Physics behind the Barrier to Internal Rotation of an Acetyl Chloride Molecule: A Combined Approach from Density Functional Theory, Car-Parrinello Molecular Dynamics, and Time-Resolved Wavelet Transform Theory

ACS Omega, (3): 6794-6803. 2018. 10.1021/acsomega.8b00316

Dutta, S.; Maity, B.; Thirumalai, D.; Koley, D.

Computational Investigation of Carbene-Phosphinidenes: Correlation between P-31 Chemical Shifts and Bonding Features to Estimate the pi-Backdonation of Carbenes

Inorganic Chemistry, (57): 3993-4008. 2018. 10.1021/acs.inorgchem.8b00174

Dzeba, I.; Bonifacic, M.; Niksic-Franjic, I.; Ljubic, I.

Proton-coupled electron transfer is the dominant mechanism of reduction of haloacetates by the -hydroxyethyl radical in aqueous media

Physical Chemistry Chemical Physics, (20): 19829-19840. 2018. 10.1039/c8cp03544j

Ebrahimi, S.; Dabbagh, H. A.; Eskandari, K.

Arrangement and nature of intermolecular hydrogen bonding in complex biomolecular systems: modeling the vitamin C---L-alanine interaction

Structural Chemistry, (29): 491-502. 2018. 10.1007/s11224-017-1046-4

Echeverria, J.

Intermolecular Carbonyl ... Carbonyl Interactions in Transition-Metal Complexes  
Inorganic Chemistry, (57): 5429-5437. 2018. 10.1021/acs.inorgchem.8b00392

Echeverria, J.

The interplay of non-covalent interactions determining the antiparallel conformation of (isocyanide)gold(I) dimers  
Crystengcomm, (20): 3987-3993. 2018. 10.1039/c8ce00616d

Echeverria, J. C.; Moriones, P.; Arzamendi, G.; Garrido, J. J.; Gil, M. J.; Cornejo, A.; Martinez-Merino, V.

Kinetics of the acid-catalyzed hydrolysis of tetraethoxysilane (TEOS) by Si-29 NMR spectroscopy and mathematical modeling

Journal of Sol-Gel Science and Technology, (86): 316-328. 2018. 10.1007/s10971-018-4637-7

Egan, C. K.; Paesani, F.

Assessing Many-Body Effects of Water Self-Ions. I: OH-(H<sub>2</sub>O)(n) Clusters

Journal of Chemical Theory and Computation, (14): 1982-1997. 2018. 10.1021/acs.jctc.7b01273

Ekennia, A. C.; Osowole, A. A.; Onwudiwe, D. C.; Babahan, I.; Ibeji, C. U.; Okafor, S. N.; Ujam, O. T.

Synthesis, characterization, molecular docking, biological activity and density functional theory studies of novel 1,4-naphthoquinone derivatives and Pd(II), Ni(II) and Co(II) complexes

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4310

El Mahdy, A. M.; Taha, H. O.; Kamel, M. A.; El Shemy, F.

Theoretical study of hydrogen storage reactions on nickel-decorated heterofullerene C-58 BX<sub>N</sub>Y (X plus Y=2)

Molecular Physics, (116): 2321-2342. 2018. 10.1080/00268976.2018.1483536

El Mandy, A. M.; Halim, S. A.; Taha, H. O.

DFT and TD-DFT calculations of metallotetraphenylporphyrin and metallotetraphenylporphyrin fullerene complexes as potential dye sensitizers for solar cells

Journal of Molecular Structure, (1160): 415-427. 2018. 10.1016/j.molstruc.2018.02.041

Elakkiya, M. T.; PremKumar, S.; Sathyendran, M.; Suresh, P.; Shanmugaiah, V.; Anitha, K.

Structural, spectral, computational, thermal and antibacterial studies on a co-crystal: 2-Aminopyrazine phthalic acid

Journal of Molecular Structure, (1173): 635-646. 2018. 10.1016/j.molstruc.2018.07.022

El-Azab, A. S.; Mary, Y. S.; Abdel-Aziz, A. A. M.; Miniyar, P. B.; Armakovic, S.; Armakovic, S. J.

Synthesis, spectroscopic analyses (FT-IR and NMR), vibrational study, chemical reactivity and molecular docking study and anti-tubercular activity of condensed oxadiazole and pyrazine derivatives  
Journal of Molecular Structure, (1156): 657-674. 2018. 10.1016/j.molstruc.2017.12.018

El-Khouly, M. E.; El-Refaey, A.; Shaban, S. Y.; El-Hendawy, M. M.  
Intramolecular electron transfer of light harvesting perylene-pyrene supramolecular conjugate  
Photochemical & Photobiological Sciences, (17): 1098-1107. 2018. 10.1039/c8pp00134k

El-Massaoudi, M.; Radi, S.; Salhi, A.; Mabkhout, Y. N.; Al>Showiman, S. S.; Ghabbour, H. A.; Adarsh, N. N.; Garcia, Y.

Novel 1D coordination polymers built from acyclic cryptate containing bis(1H-1,2,4-triazole) ligands and featuring coordinated counteranions  
New Journal of Chemistry, (42): 11324-11333. 2018. 10.1039/c8nj00799c

El-Meligy, A. B.; Koga, N.; Iuchi, S.; Yoshida, K.; Hirao, K.; Mangood, A. H.; El-Nahas, A. M.  
DFT/TD-DFT calculations of the electronic and optical properties of bis-N,N-dimethylaniline-based dyes for use in dye-sensitized solar cells  
Journal of Photochemistry and Photobiology a-Chemistry, (367): 332-346. 2018.  
10.1016/j.jphotochem.2018.08.036

El-Shafiy, H. F.; Shebl, M.  
Oxovanadium(IV), cerium(III), thorium(IV) and dioxouranium(VI) complexes of 1-ethyl-4-hydroxy-3-(nitroacetyl)quinolin-2(1H)-one: Synthesis, spectral, thermal, fluorescence, DFT calculations, antimicrobial and antitumor studies  
Journal of Molecular Structure, (1156): 403-417. 2018. 10.1016/j.molstruc.2017.11.081

Emamian, S.; Lu, T.; Domingo, L. R.; Saremi, L. H.; Rios-Gutierrez, M.  
A molecular electron density theory study of the chemo- and regioselective 3+2 cycloaddition reactions between trifluoroacetonitrile N-oxide and thioketones  
Chemical Physics, (501): 128-137. 2018. 10.1016/j.chemphys.2017.12.019

Engelhardt, F.; Maass, C.; Andrade, D. M.; Herbst-Irmer, R.; Stalke, D.  
Benchmarking lithium amide versus amine bonding by charge density and energy decomposition analysis arguments  
Chemical Science, (9): 3111-3121. 2018. 10.1039/c7sc05368a

Escudero-Adan, E. C.; Bauza, A.; Lecomte, C.; Frontera, A.; Ballester, P.  
Boron triel bonding: a weak electrostatic interaction lacking electron-density descriptors  
Physical Chemistry Chemical Physics, (20): 24192-24200. 2018. 10.1039/c8cp04401e

Eskandari, K.; Ebadinejad, F.  
Metal-ligand bond directionality in the M-2-NH<sub>3</sub> complexes (M = Cu, Ag and Au)  
Molecular Physics, (116): 1369-1376. 2018. 10.1080/00268976.2018.1431408

Esme, A.; Sagdinc, S. G.

Molecular structures, spectroscopic (FT-IR, NMR, UV) studies, NBO analysis and NLO properties for tautomeric forms of 1,3-dimethyl-5-(phenylazo)-6-aminouracil by density functional method

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (188): 443-455. 2018.

10.1016/j.saa.2017.07.034

Espada, M. F.; Esqueda, A. C.; Campos, J.; Rubio, M.; Lopez-Serrano, J.; Alvarez, E.; Maya, C.; Carmona, E.

Cationic ( $\eta$ (5)-C<sub>5</sub>Me<sub>4</sub>R)Rh-III Complexes with Metalated Aryl Phosphines Featuring  $\eta$ (4)-Phosphorus plus Pseudo-Allylic Coordination

Organometallics, (37): 11-21. 2018. 10.1021/acs.organomet.7b00688

Espinosa-Hicks, C.; Montoya, P.; Bautista, R.; Jimenez-Vazquez, H. A.; Rodriguez-Valdez, L. M.; Camacho-Davila, A. A.; Cossio, F. P.; Delgado, F.; Tamariz, J.

Synthesis of exo-Imidazolidin-2-one Dienes, Their Isomerization, and Selectivity in Diels-Alder Cycloadditions

Journal of Organic Chemistry, (83): 5347-5364. 2018. 10.1021/acs.joc.7b02344

Esrafili, M. D.; Abdollahpour, H.; Saeidi, N.

Metal-Free Reduction of NO over a Fullerene-like Boron Nitride Nanocluster: A Mechanistic Study by DFT Calculations

Chemistryselect, (3): 1168-1175. 2018. 10.1002/slct.201702812

Esrafili, M. D.; Asadollahi, S.; Mousavian, P.

Anionic tetrel bonds: An ab initio study

Chemical Physics Letters, (691): 394-400. 2018. 10.1016/j.cplett.2017.11.051

Esrafili, M. D.; Asadollahi, S.; Mousavian, P.

Exploring hydride-pi interactions and their tuning by sigma-hole bonds: an ab initio study

Molecular Physics, (116): 118-128. 2018. 10.1080/00268976.2017.1369186

Esrafili, M. D.; Dinparast, L.

The selective adsorption of formaldehyde and methanol over Al- or Si-decorated graphene oxide: A DFT study

Journal of Molecular Graphics & Modelling, (80): 25-31. 2018. 10.1016/j.jmgm.2017.12.025

Esrafili, M. D.; Heydari, S.

Carbon-doped boron-nitride fullerenes as efficient metal-free catalysts for oxidation of SO<sub>2</sub>: a DFT study

Structural Chemistry, (29): 275-283. 2018. 10.1007/s11224-017-1027-7

Esrafili, M. D.; Mousavian, P.

The strengthening effect of a halogen, chalcogen or pnicogen bonding on halogen-pi interaction: a comparative ab initio study

Molecular Physics, (116): 526-535. 2018. 10.1080/00268976.2017.1406166

Esrafili, M. D.; Mousavian, P.

Strong Tetrel Bonds: Theoretical Aspects and Experimental Evidence  
Molecules, (23) 2018. 10.3390/molecules23102642

Esrafili, M. D.; Mousavian, P.

The triel bond: a potential force for tuning anion-pi interactions  
Molecular Physics, (116): 388-398. 2018. 10.1080/00268976.2017.1393118

Esrafili, M. D.; Sadr-Mousavi, A.

A computational study on the strength and nature of bifurcated aerogen bonds  
Chemical Physics Letters, (698): 1-6. 2018. 10.1016/j.cplett.2018.02.066

Esrafili, M. D.; Vessally, E.

N<sub>2</sub>O + CO reaction over single Ga or Ge atom embedded graphene: A DFT study  
Surface Science, (667): 105-111. 2018. 10.1016/j.susc.2017.10.001

Esseffar, M.; Parish, C. A.; Jala, R.; Lamsabhi, A. M.

A Computational Study of the Reactivity of 3,5-(Oxo/Thioxo) Derivatives of 2,7-Dimethyl-1,2,4-Triazepines. Keto-Enol Tautomerization and Potential for Hydrogen Storage  
Journal of Physical Chemistry A, (122): 3076-3086. 2018. 10.1021/acs.jpca.8b00251

Fallah, N.; Gholivand, K.; Yousefi, M.; Azar, P. A.

Synthesis, spectroscopic characterization, anti-urease activities of a novel bisphosphoramidate, a combined experimental and computational study  
Journal of Molecular Structure, (1173): 801-813. 2018. 10.1016/j.molstruc.2018.06.106

Falvey, D. E.

Discrete Existence of Singlet Nitrenium Ions Revisited: Computational Studies of Non-Aryl Nitrenium Ions and Their Rearrangements  
ACS Omega, (3): 10418-10432. 2018. 10.1021/acsomega.8b01038

Fan, Q. W.; Li, P.; Yan, H.

Photophysical properties of 2,6-unsubstituted 1,4-dihydropyridines: Experimental and theoretical studies  
Journal of Photochemistry and Photobiology a-Chemistry, (358): 51-60. 2018.  
10.1016/j.jphotochem.2018.03.009

Fang, Z. T.; Garner, E. B.; Dixon, D. A.; Gong, Y.; Andrews, L.; Liebov, B.

Laser-Ablated U Atom Reactions with (CN)(2) to Form UNC, U(NC)(2), and U(NC)(4): Matrix Infrared Spectra and Quantum Chemical Calculations  
Journal of Physical Chemistry A, (122): 516-528. 2018. 10.1021/acs.jpca.7b09291

Farhat, D.; Maibach, J.; Eriksson, H.; Edstrom, K.; Lemordant, D.; Ghamouss, F.

Towards high-voltage Li-ion batteries: Reversible cycling of graphite anodes and Li-ion batteries in adiponitrile-based electrolytes

Electrochimica Acta, (281): 299-311. 2018. 10.1016/j.electacta.2018.05.133

Farkhani, E. T.; Pourayoubi, M.; Izadyar, M.; Andreev, P. V.; Shchegrevina, E. S.

Evaluation of N-H center dot center dot center dot S and N-H center dot center dot center dot pi interactions in O,O'-diethyl N-(2,4,6-trimethylphenyl)thiophosphate: a combination of X-ray crystallographic and theoretical studies

Acta Crystallographica Section C-Structural Chemistry, (74): 847-+. 2018.

10.1107/s2053229618007933

Farrokhpour, H.; Ghandehari, M.; Eskandari, K.

ONIOM DFT study of the adsorption of cytosine on the Au/Ag and Ag/Au bimetallic nanosurfaces: The effect of sublayer

Applied Surface Science, (457): 712-725. 2018. 10.1016/j.apsusc.2018.06.279

Fatma, S.; Bishnoi, A.; Verma, A. K.; Singh, V.; Srivastava, K.

Quantum chemical calculations and molecular docking studies of 5-(4-chlorobenzylidene)thiazolidine-2,4-dione(CTD) and its mannich product 5-(4-chlorobenzylidene)-3-(morpholinomethyl)thiazolidine-2,4-dione (CMTD)

Journal of Molecular Structure, (1157): 177-190. 2018. 10.1016/j.molstruc.2017.12.051

Fatma, S.; Parveen, H.; Bishnoi, A.; Verma, A. K.; Srivastava, K.

Molecular orbital, spectroscopic, first order hyperpolarizability and NBO analysis of aryl-substituted 5-(benzylidene) thiazolidine-2,4-diones

Indian Journal of Pure & Applied Physics, (56): 491-508. 2018.

Fedik, N.; Boldyrev, A. I.

Insight into The Nature of Rim Bonds in Coronene

Journal of Physical Chemistry A, (122): 8585-8590. 2018. 10.1021/acs.jpca.8b07937

Fedorova, I. V.; Safanova, L. P.

Influence of Cation Size on the Structural Features and Interactions in Tertiary Alkylammonium Trifluoroacetates: A Density Functional Theory Investigation

Journal of Physical Chemistry A, (122): 5878-5885. 2018. 10.1021/acs.jpca.8b04003

Fedorova, I. V.; Safanova, L. P.

The Nature of the Interactions in Triethanolammonium-Based Ionic Liquids. A Quantum Chemical Study

Journal of Physical Chemistry A, (122): 4562-4570. 2018. 10.1021/acs.jpca.8b02598

Fei, T.; Du, Y.; He, C. L.; Pang, S. P.

Theoretical investigations on azole-fused tricyclic 1,2,3,4-tetrazine-2-oxides

RSC Advances, (8): 27235-27245. 2018. 10.1039/c8ra05274c

Feichtner, K. S.; Scherpf, T.; Gessner, V. H.

Cooperative Bond Activation Reactions with Ruthenium Carbene Complex

PhSO<sub>2</sub>(Ph<sub>2</sub>PNSiMe<sub>3</sub>)C=Ru(p-cymene): Ru=C and N-Si Bond Reactivity

Organometallics, (37): 645-654. 2018. 10.1021/acs.organomet.7b00254

Feijoo, M. G.; Fernandez-Liencres, M. P.; Gil, D. M.; Gomez, M. I.; Ben Altabef, A.; Navarro, A.; Tuttolomondo, M. E.

A detailed study of intermolecular interactions, electronic and vibrational properties of the metal complex bis(uracilato)diammine copper(ii) dihydrate

Journal of Molecular Structure, (1155): 424-433. 2018. 10.1016/j.molstruc.2017.11.030

Felscia, U. R.; Rajkumar, B. J. M.; Nidya, M.; Sankar, P.

Electronic and Nonlinear Optical Properties of L-Histidine on Silver: A Theoretical and Experimental Approach

Journal of Physical Chemistry A, (122): 1045-1052. 2018. 10.1021/acs.jpca.7b07493

Feng, L. Y.; Guo, J. C.; Li, P. F.; Zhai, H. J.

Boron-based binary Be<sub>6</sub>B<sub>10</sub>- cluster: three-layered aromatic sandwich, electronic transmutation, and dynamic structural fluxionality

Physical Chemistry Chemical Physics, (20): 22719-22729. 2018. 10.1039/c8cp04332a

Feng, Y.; Zhang, Y. L.; Du, G. X.; Zhang, J. B.; Qu, X. H.

Experimental and first-principles study of a metal-organic framework with sulfur embedding cathode for enhanced performance lithium-sulfur battery

Sustainable Energy & Fuels, (2): 1828-1836. 2018. 10.1039/c8se00195b

Feng, Z. C.; Zhang, H.; Xu, K. Z.; Song, J. R.; Zhao, F. Q.

Six new complexes constructed from silver(I) and 2-(dinitromethylene)-1,3-diazacyclopentane (DNDZ): Synthesis, crystal structure and properties

Journal of Molecular Structure, (1158): 255-263. 2018. 10.1016/j.molstruc.2018.01.036

Fereidoni, S.; Ghiasi, R.; Pasdar, H.

Theoretical Study of the Solvent Effect on the Electronic and Vibrational Properties of CpFe(CO)(2)(NCS) and CpFe(CO)(2)(SCN) Linkage Isomers

Journal of Structural Chemistry, (59): 1058-1066. 2018. 10.1134/s0022476618050074

Fianchini, M.; Bandeira, N. A. G.

Are homoleptic complexes of ethylene with group 12 metals isolable in solution? A DFT study

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3683-y

Firouzbakht, M.; Rijs, N. J.; Schlangen, M.; Kaupp, M.; Schwarz, H.

Ligand Effects on the Reactivity of CoX (+) (X = CN, F, Cl, Br, O, OH) Towards CO<sub>2</sub>: Gas-Phase Generation of the Elusive Cyanoformate by Co(CN) (+) and Fe(CN) (+)

Topics in Catalysis, (61): 575-584. 2018. 10.1007/s11244-018-0903-8

Fisher, G.; Thomson, C. M.; Stroek, R.; Czekster, C. M.; Hirschi, J. S.; da Silva, R. G.

Allosteric Activation Shifts the Rate-Limiting Step in a Short-Form ATP

Phosphoribosyltransferase

Biochemistry, (57): 4357-4367. 2018. 10.1021/acs.biochem.8b00559

Fitch, R. W.; Snider, B. B.; Zhou, Q.; Foxman, B. M.; Pandya, A. A.; Yakel, J. L.; Olson, T. T.; Al-Muhtasib, N.; Xiao, Y. X.; Welch, K. D.; Panter, K. E.

Absolute Configuration and Pharmacology of the Poison Frog Alkaloid Phantasmidine

Journal of Natural Products, (81): 1029-1035. 2018. 10.1021/acs.jnatprod.8b00062

Fizer, O.; Fizer, M.; Sidey, V.; Studenyak, Y.; Mariychuk, R.

Benchmark of different charges for prediction of the partitioning coefficient through the hydrophilic/lipophilic index

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3692-x

Flores, M. C.; Marquez, E. A.; Mora, J. R.

Molecular modeling studies of bromopyrrole alkaloids as potential antimalarial compounds: a DFT approach

Medicinal Chemistry Research, (27): 844-856. 2018. 10.1007/s00044-017-2107-3

Flores, R.; Reyes-Garcia, L. I.; Rodriguez-Laguna, N.; Gomez-Balderas, R.

Stability constants of Cu(II)/indomethacin mononuclear complexes in solution

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2315-z

Florez, E.; Acelas, N.; Ramirez, F.; Hadad, C.; Restrepo, A.

Microsolvation of F

Physical Chemistry Chemical Physics, (20): 8909-8916. 2018. 10.1039/c8cp00819a

Fogarty, R. M.; Matthews, R. P.; Ashworth, C. R.; Brandt-Talbot, A.; Palgrave, R. G.; Bourne, R. A.; Hoogerstraete, T. V.; Hunt, P. A.; Lovelock, K. R. J.

Experimental validation of calculated atomic charges in ionic liquids

Journal of Chemical Physics, (148) 2018. 10.1063/1.5011662

Fogarty, R. M.; Rowe, R.; Matthews, R. P.; Clough, M. T.; Ashworth, C. R.; Brandt, A.; Corbett, P. J.; Palgrave, R. G.; Smith, E. F.; Bourne, R. A.; Chamberlain, T. W.; Thompson, P. B. J.; Hunt, P. A.; Lovelock, K. R. J.

Atomic charges of sulfur in ionic liquids: experiments and calculations

Faraday Discussions, (206): 183-201. 2018. 10.1039/c7fd00155j

Fominykh, O. D.; Kalinin, A. A.; Sharipova, S. M.; Sharipova, A. V.; Burganov, T. I.; Smirnov, M. A.; Vakhonina, T. A.; Levitskaya, A. I.; Kadyrova, A. A.; Ivanova, N. V.; Khamatgalimov, A. R.; Nizameev, I. R.; Katsyuba, S. A.; Balakina, M. Y.

Composite materials containing chromophores with 3,7-(di) vinylquinoxalinone pi-electron bridge doped into PMMA: Atomistic modeling and measurements of quadratic nonlinear optical activity  
Dyes and Pigments, (158): 131-141. 2018. 10.1016/j.dyepig.2018.05.033

Foretic, B.; Vianello, R.; Matkovic-Calogovic, D.; Jadresko, D.; Picek, I.  
Supramolecular inter-ionic charge-transfer complexes between derivatives of pyridinium-4-oxime cations and hexacyanoferrate(II) anions  
New Journal of Chemistry, (42): 16115-16126. 2018. 10.1039/c8nj03066a

Foroutan-Nejad, C.; Straka, M.; Fernandez, I.; Frenking, G.  
Buckyball Difluoride F-2(-)@C-60(+)-A Single-Molecule Crystal  
Angewandte Chemie-International Edition, (57): 13931-13934. 2018. 10.1002/anie.201809699

Fouegue, A. D. T.; Mama, D. B.; Ghogomu, J. N.; Elie, Y.; Etoh, M. A.  
The Substitution Effect on Reaction Enthalpies of Antioxidant Mechanisms of Juglone and Its Derivatives in Gas and Solution Phase: DFT Study  
Journal of Chemistry, 2018. 10.1155/2018/1958047

Franco, J. H.; da Silva, B. F.; Oliveira, R. V.; Meireles, G.; de Oliveira, D. P.; de Castro, A. A.; Ramalho, T. C.; Zanoni, M. V. B.  
Identification of biotransformation products of disperse dyes with rat liver microsomes by LC-MS/MS and theoretical studies with DNA: Structure-mutagenicity relationship using Salmonella/microsome assay  
Science of the Total Environment, (613): 1093-1103. 2018. 10.1016/j.scitotenv.2017.08.271

Franski, R.; Gierczyk, B.; Zalas, M.; Jankowski, W.; Hoffmann, M.  
Methyl group transfer upon gas phase decomposition of protonated methyl benzoate and similar compounds  
Journal of Mass Spectrometry, (53): 379-384. 2018. 10.1002/jms.4069

Freindorf, M.; Cremer, D.; Kraka, E.  
Gold(I)-assisted catalysis - a comprehensive view on the 3,3 -sigmatropic rearrangement of allyl acetate  
Molecular Physics, (116): 611-630. 2018. 10.1080/00268976.2017.1382735

Freitas, V. L. S.; da Silva, M.  
Influence of Hydroxyl Functional Group on the Structure and Stability of Xanthone: A Computational Approach  
Molecules, (23) 2018. 10.3390/molecules23112962

Freitas, V. L. S.; Ferreira, P. J. O.; da Silva, M.  
Experimental and computational thermochemical studies of acridone and N-methylacridone  
Journal of Chemical Thermodynamics, (118): 115-126. 2018. 10.1016/j.jct.2017.11.002

Friedrich, J.; Qiao, Y. S.; Maichle-Mossmer, C.; Schelter, E. J.; Anwander, R.  
Redox-enhanced hemilability of a tris(tert-butoxy) siloxy ligand at cerium  
*Dalton Transactions*, (47): 10113-10123. 2018. 10.1039/c8dt01878b

Frontera, A.; Bauza, A.  
Regium-pi bonds: An Unexplored Link between Noble Metal Nanoparticles and Aromatic Surfaces  
*Chemistry-a European Journal*, (24): 7228-7234. 2018. 10.1002/chem.201800820

Frontera, A.; Bauza, A.  
Sn Tetrel Bonds in the Activation of Peroxisome Proliferator-Activated Receptors (PPARs) by Organotin Molecules  
*Chemistry-a European Journal*, (24): 16582-16587. 2018. 10.1002/chem.201804676

Fu, C.; Zhang, G. S.; Wang, H. Y.; Li, L.; Fu, J. W.; Sun, Y. N.; Zhang, H.  
Different photochromic properties induced by lone pair- interactions with varying strengths in two stereocontrolled self-assembly isomeric coordination polymers  
*Crystengcomm*, (20): 6821-6827. 2018. 10.1039/c8ce01367e

Fu, L. J.; Mu, X. L.; Li, B. Q.  
Reaction mechanism of organoselenium-catalyzed syn-dichlorination of alkenes: a DFT study  
*Journal of Molecular Modeling*, (24) 2018. 10.1007/s00894-018-3624-9

Fugel, M.; Beckmann, J.; Jayatilaka, D.; Gibbs, G. V.; Grabowsky, S.  
A Variety of Bond Analysis Methods, One Answer? An Investigation of the Element-Oxygen Bond of Hydroxides H<sub>n</sub>XOH  
*Chemistry-a European Journal*, (24): 6248-6261. 2018. 10.1002/chem.201800453

Fugel, M.; Hesse, M. F.; Pal, R.; Beckmann, J.; Jayatilaka, D.; Turner, M. J.; Karton, A.; Bultinck, P.; Chandler, G. S.; Grabowsky, S.  
Covalency and Ionicity Do Not Oppose Each Other-Relationship Between Si-O Bond Character and Basicity of Siloxanes  
*Chemistry-a European Journal*, (24): 15275-15286. 2018. 10.1002/chem.201802197

Fugel, M.; Kleemiss, F.; Malaspina, L. A.; Pal, R.; Spackman, P. R.; Jayatilaka, D.; Grabotvsky, S.  
Investigating the Resonance in Nitric Acid and the Nitrate Anion Based on a Modern Bonding Analysis  
*Australian Journal of Chemistry*, (71): 227-237. 2018. 10.1071/ch17583

Fujimori, S.; Mizuhata, Y.; Tokitoh, N.  
Ru-Complexes of an anionic germabenzenyl ligand  
*Chemical Communications*, (54): 8044-8047. 2018. 10.1039/c8cc02845a

Fujimori, S.; Mizuhata, Y.; Tokitoh, N.

Stannabenzylpotassium: The First Isolable Tin-Containing Benzene Derivative  
Chemistry-a European Journal, (24): 17039-17045. 2018. 10.1002/chem.201804858

Fukazawa, A.; Toda, Y.; Hayakawa, M.; Sekioka, A.; Ishii, H.; Okamoto, T.; Takeya, J.; Hijikata, Y.; Yamaguchi, S.

End-Capping pi-Conjugated Systems with Medium-Sized Sulfur-Containing Rings: A Route Towards Solution-Processable Air-Stable Semiconductors

Chemistry-a European Journal, (24): 11503-11510. 2018. 10.1002/chem.201802656

Fukuda, R.; Sakai, S.; Takagi, N.; Matsui, M.; Ehara, M.; Hosokawa, S.; Tanaka, T.; Sakaki, S.

Mechanism of NO-CO reaction over highly dispersed cuprous oxide on gamma-alumina catalyst using a metal-support interfacial site in the presence of oxygen: similarities to and differences from biological systems

Catalysis Science & Technology, (8): 3833-3845. 2018. 10.1039/c8cy00080h

Funaki, C.; Yamamoto, S.; Hoshina, H.; Ozaki, Y.; Sato, H.

Three different kinds of weak C-H center dot center dot center dot O=C inter- and intramolecular interactions in poly(epsilon-caprolactone) studied by using terahertz spectroscopy, infrared spectroscopy and quantum chemical calculations

Polymer, (137): 245-254. 2018. 10.1016/j.polymer.2018.01.025

Furer, V. L.; Potapova, L. I.; Vatsouro, I. M.; Kovalev, V. V.; Shokova, E. A.; Kovalenko, V. I.

Investigation of the conformation and hydrogen bonds in adamantlylthiacalix 4 arene by IR spectroscopy and DFT

Journal of Molecular Structure, (1171): 207-213. 2018. 10.1016/j.molstruc.2018.06.008

Furer, V. L.; Potapova, L. I.; Vatsouro, I. M.; Kovalev, V. V.; Shokova, E. A.; Kovalenko, V. I.

Investigation of the structure and hydrogen bonds in adamantlylcalix 6 arene by IR spectroscopy and DFT

Vibrational Spectroscopy, (96): 60-66. 2018. 10.1016/j.vibspec.2018.03.003

Furer, V. L.; Vandyukov, A. E.; Majoral, J. P.; Caminade, A. M.; Gottis, S.; Laurent, R.; Kovalenko, V. I.

Vibrational spectroscopic investigation of the gold complexation within the cascade structure of phosphorus-containing dendrimer

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (203): 118-126. 2018. 10.1016/j.saa.2018.05.111

Furer, V. L.; Vandyukov, A. E.; Tripathi, V.; Majoral, J. P.; Caminade, A. M.; Kovalenko, V. I.

Vibrational spectroscopic study of cationic phosphorus dendrimers with aminoethylpiperidine terminal groups

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (194): 211-221. 2018. 10.1016/j.saa.2018.01.031

Furer, V. L.; Vandyukov, A. E.; Zaripov, S. R.; Solovieva, S. E.; Antipin, I. S.; Kovalenko, V. I.

FT-IR and FT-Raman study of hydrogen bonding in p-alkylcalix 8 arenes  
Vibrational Spectroscopy, (95): 38-43. 2018. 10.1016/j.vibspec.2018.01.006

Galabov, B.; Koleva, G.; Schaefer, H. F.; Allen, W. D.  
Nucleophilic Influences and Origin of the S(N)2 Allylic Effect  
Chemistry-a European Journal, (24): 11637-11648. 2018. 10.1002/chem.201801187

Galley, S. S.; Arico, A. A.; Lee, T. H.; Deng, X. Y.; Yao, Y. X.; Sperling, J. M.; Proust, V.; Storbeck, J. S.; Dobrosavljevic, V.; Neu, J. N.; Siegrist, T.; Baumbach, R. E.; Albrecht-Schmitt, T. E.; Kaltsoyannis, N.; Lanata, N.

Uncovering the Origin of Divergence in the CsM(CrO<sub>4</sub>)<sub>2</sub> (M = La, Pr, Nd, Sm, Eu; Am) Family through Examination of the Chemical Bonding in a Molecular Cluster and by Band Structure Analysis  
Journal of the American Chemical Society, (140): 1674-1685. 2018. 10.1021/jacs.7b09474

Galvan, J. E.; Lestard, M. E. D.; Piro, O. E.; Echeverria, G.; Molina, R. D. I.; Arena, M. E.; Ulic, S. E.; Tuttolomondo, M. E.; Ben Altabef, A.

Synthesis, characterization and crystal structure of 2-chloroethyl(methylsulfonyl)methanesulfonate  
New Journal of Chemistry, (42): 11073-11084. 2018. 10.1039/c7nj05138g

Ganesamoorthy, C.; Kruger, J.; Glockler, E.; Helling, C.; John, L.; Frank, W.; Wolper, C.; Schulz, S.  
Comprehensive Study on Reactions of Group 13 Diyls with Tetraorganodipentelanes  
Inorganic Chemistry, (57): 9495-9503. 2018. 10.1021/acs.inorgchem.8b01489

Ganesan, M.; Vedamanickam, N.; Paranthaman, S.  
Studies of intramolecular H-bond interactions and solvent effects in the conformers of glycolic acid - A quantum chemical study  
Journal of Theoretical & Computational Chemistry, (17) 2018. 10.1142/s0219633618500098

Gangadharan, R. P.; Krishnan, S. S.  
Quantum Chemical Calculations on 4- 2-(Tert-Butylamino)-1-Hydroxyethyl -2-(Hydroxymethyl) Phenol by Density Functional Theory  
Spectroscopy and Spectral Analysis, (38): 3631-3637. 2018. 10.3964/j.issn.1000-0593(2018)11-3631-07

Gani, T. Z. H.; Kulik, H. J.  
Understanding and Breaking Scaling Relations in Single-Site Catalysis: Methane to Methanol Conversion by Fe-IV=O  
ACS Catalysis, (8): 975-986. 2018. 10.1021/acscatal.7b03597

Gao, K. Q.; Sheng, L.  
Neutral noble gas compound with a xenon-metal double bond: A theoretical study of F<sub>2</sub>XeWF<sub>2</sub>  
Computational and Theoretical Chemistry, (1123): 35-40. 2018. 10.1016/j.comptc.2017.10.018

Gao, N.; Lin, X. C.; Liu, J. L.; Li, Y. Z.; Yang, Y. H.  
Photoactuated Properties of Acetylene-Congeners Non-Metallic Dyes and Molecular Design for  
Solar Cells  
Materials, (11) 2018. 10.3390/ma11102027

Gao, X. Z.; Li, N.; King, R. B.  
Heterometallic bonding between a first row transition metal and a third row transition metal:  
The cyclopentadienyliron rhenium carbonyls CpFeRe(CO)(n) (n=7, 6, 5)  
Polyhedron, (145): 231-238. 2018. 10.1016/j.poly.2017.10.001

Garcia-Calvo, J.; Calvo-Gredilla, P.; Ibanez-Llorente, M.; Romero, D. C.; Cuevas, J. V.; Garcia-Herbosa, G.; Avella, M.; Torroba, T.

Surface functionalized silica nanoparticles for the off-on fluorogenic detection of an improvised explosive, TATP, in a vapour flow

Journal of Materials Chemistry A, (6): 4416-4423. 2018. 10.1039/c7ta10792g

Garcia-Reyes, F.; Fantoni, A. C.; Baron, M.; Romano, R. M.; Punte, G. M.; Echeverria, G. A.  
Role of weak C-H center dot center dot center dot O and strong N-H center dot center dot center dot O intermolecular interactions on the high-symmetry molecular packing of trans-cyclohexane-1,4-dicarboxamide

Acta Crystallographica Section C-Structural Chemistry, (74): 1068-. 2018.  
10.1107/s2053229618011750

Gatfaoui, S.; Issaoui, N.; Brandan, S. A.; Roisnel, T.; Marouani, H.  
Synthesis and characterization of p-xylylenediaminium bis(nitrate). Effects of the coordination modes of nitrate groups on their structural and vibrational properties  
Journal of Molecular Structure, (1151): 152-168. 2018. 10.1016/j.molstruc.2017.09.027

Gaudin, T.; Fayet, G.; Rotureau, P.; Pezron, I.  
Anticipating Dissolution Issues of Sugar-Based Surfactants through a Decision Tree Approach  
Journal of Surfactants and Detergents, (21): 835-843. 2018. 10.1002/jsde.12178

Gaudin, T.; Rotureau, P.; Pezron, I.; Fayet, G.  
Investigating the impact of sugar-based surfactants structure on surface tension at critical micelle concentration with structure-property relationships  
Journal of Colloid and Interface Science, (516): 162-171. 2018. 10.1016/j.jcis.2018.01.051

Gawale, Y.; Sekar, N.  
Investigating the excited state optical properties and origin of large stokes shift in Benz c,d indole N-Heteroarene BF<sub>2</sub> dyes with ab initio tools  
Journal of Photochemistry and Photobiology B-Biology, (178): 472-480. 2018.  
10.1016/j.jphotobiol.2017.12.006

Geboes, Y.; De Vos, E.; Herrebout, W. A.

S center dot center dot center dot S and S center dot center dot center dot P chalcogen bonding in solution: a cryospectroscopic study of the complexes of 2,2,4,4-tetrafluoro-1,3-dithietane with dimethyl sulfide and trimethylphosphine

New Journal of Chemistry, (42): 10563-10571. 2018. 10.1039/c8nj01648h

Geeson, M. B.; Cummins, C. C.

Phosphoric acid as a precursor to chemicals traditionally synthesized from white phosphorus  
Science, (359): 1383-1385. 2018. 10.1126/science.aar6620

Geng, S.; Liu, Y. Y.; Xue, Y.

Gas-phase alkyl and N-alkylamino cation affinities of anionic alpha-oxygen nucleophiles ( $H_nXO^-$ ;  $X = N, P, As, O, S, Se, F, Cl, Br; n=0-2$ ): a theoretical G2(+)(M) study

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-017-3531-5

Geng, S.; Sang, X. L.; Liu, X. Q.; Ren, Y.; Xue, Y.

A theoretical study of UV-Vis spectrum and antioxidant activity of chryso-obtusin

Journal of Theoretical & Computational Chemistry, (17) 2018. 10.1142/s0219633618500153

Genoni, A.; Bucinsky, L.; Claiser, N.; Contreras-Garcia, J.; Dittrich, B.; Dominiak, P. M.; Espinosa, E.; Gatti, C.; Giannozzi, P.; Gillet, J. M.; Jayatilaka, D.; Macchi, P.; Madsen, A. O.; Massa, L.; Matta, C. F.; Merz, K. M.; Nakashima, P. N. H.; Ott, H.; Ryde, U.; Schwarz, K.; Sierka, M.; Grabowsky, S.

Quantum Crystallography: Current Developments and Future Perspectives

Chemistry-a European Journal, (24): 10881-10905. 2018. 10.1002/chem.201705952

Georg, I.; Teichmann, J.; Bursch, M.; Tillmann, J.; Endeward, B.; Bolte, M.; Lerner, H. W.; Grimme, S.; Wagner, M.

Exhaustively Trichlorosilylated C-1 and C-2 Building Blocks: Beyond the Muller-Rochow Direct Process

Journal of the American Chemical Society, (140): 9696-9708. 2018. 10.1021/jacs.8b05950

George, J.; Prasana, J. C.; Muthu, S.; Kuruvilla, T. K.; Sevanthi, S.; Saji, R. S.

Spectroscopic (FT-IR, FT Raman) and quantum mechanical study on N-(2,6-dimethylphenyl)-2-{4- 2-hydroxy-3-(2-methoxyphenoxy)propyl pipera zin-1-yl)acetamide

Journal of Molecular Structure, (1171): 268-278. 2018. 10.1016/j.molstruc.2018.05.106

George, J.; Sajan, D.; Alex, J.; Aravind, A.; Vinitha, G.; Chitra, R.

An experimental and computational approach to electronic and optical properties of Diglycine barium chloride monohydrate crystal: Applications to NLO and OLED

Optics and Laser Technology, (105): 207-220. 2018. 10.1016/j.optlastec.2018.02.056

Gerber, I. C.; Poteau, R.

Critical assessment of charge transfer estimates in non-covalent graphene doping

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2365-2

Gerbig, D.; Desch, S.; Schreiner, P. R.  
Making Glycine Methyl Ester Chiral  
Chemistry-a European Journal, (24): 11904-11907. 2018. 10.1002/chem.201802119

Geri, J. B.; York, J. T.  
A systematic examination of ligand basicity effects on bonding in palladium (0)- and palladium(II)-ethylene complexes  
Inorganica Chimica Acta, (483): 191-202. 2018. 10.1016/j.ica.2018.08.008

Geronimo, I.; Payne, C. M.; Sandgren, M.  
Hydrolysis and Transglycosylation Transition States of Glycoside Hydrolase Family 3 beta-Glucosidases Differ in Charge and Puckering Conformation  
Journal of Physical Chemistry B, (122): 9452-9459. 2018. 10.1021/acs.jpcb.8b07118

Gershoni-Poranne, R.  
Piecing it Together: An Additivity Scheme for Aromaticity using NICS-XY Scans  
Chemistry-a European Journal, (24): 4165-4172. 2018. 10.1002/chem.201705407

Getmanskii, I. V.; Minyaev, R. M.; Koval, V. V.; Minkin, V. I.  
Quantum chemical modeling of solid-state B<sub>4</sub>X structures containing tetrahedral B-4 units with X = B, C, Al, Si  
Mendeleev Communications, (28): 173-175. 2018. 10.1016/j.mencom.2018.03.021

Ghana, P.; Arz, M. I.; Chakraborty, U.; Schnakenburg, G.; Filippou, A. C.  
Linearly Two-Coordinated Silicon: Transition Metal Complexes with the Functional Groups M Si-M and M=Si=M  
Journal of the American Chemical Society, (140): 7187-7198. 2018. 10.1021/jacs.8b02902

Ghana, P.; Arz, M. I.; Schnakenburg, G.; Strassmann, M.; Filippou, A. C.  
Metal-Silicon Triple Bonds: Access to Si(eta(5)-C<sub>5</sub>Me<sub>5</sub>) (+) from SiX<sub>2</sub>(NHC) and its Conversion to the Silylidyne Complex (Tp(Me)(CO)(2)MoSi(eta(3)-C<sub>5</sub>Me<sub>5</sub>) (Tp(Me) = kappa(3)-N,N',N'' -hydridotris(3,5-dimethyl-1-pyrazolyl)borate)  
Organometallics, (37): 772-780. 2018. 10.1021/acs.organomet.7b00665

Ghara, M.; Chattaraj, P. K.  
Bonding and Reactivity in RB-AsR Systems (R = H, F, OH, CH<sub>3</sub>, CMe<sub>3</sub>, CF<sub>3</sub>, SiF<sub>3</sub>, BO): Substituent Effects  
Acta Physico-Chimica Sinica, (34): 201-207. 2018. 10.3866/pku.Whxb201707131

Ghara, M.; Chattaraj, P. K.  
A DFT study on trapping of nitric oxide by 1,3,2,5-diazadiborinine, a frustrated Lewis pair  
Journal of the Indian Chemical Society, (95): 1019-1024. 2018.

Ghara, M.; Chattaraj, P. K.

Fixation of nitrous oxide (N<sub>2</sub>O) by 1, 4, 2, 5-diazadiborinine: A DFT study  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25593

Ghashghaei, M.; Ghambanian, M.

Ethene Protonation Over Silica-Grafted Metal (Cr, Mo, and W) Oxide Catalysts: A Comparative Nanocluster Modeling Study

Russian Journal of Inorganic Chemistry, (63): 1570-1577. 2018. 10.1134/s0036023618160015

Ghashghaei, M.; Ghambanian, M.

Initiation of heterogeneous Schrock-type Mo and W oxide metathesis catalysts: A quantum thermochemical study

Computational Materials Science, (155): 197-208. 2018. 10.1016/j.commatsci.2018.08.031

Ghazvini, S.; Safari, P.; Mobinikhalehi, A.; Moghanian, H.; Rasouli, H.

Synthesis, characterization, anti-diabetic potential and DFT studies of 7-hydroxy-4-methyl-2-oxo-2H-chromene-8-carbaldehyde oxime

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (205): 111-131. 2018. 10.1016/j.saa.2018.07.009

Ghiassi, H.; Raissi, H.; Marvi, M.

Boosting BeONT Reactivity with HCN by Calcium and Magnesium Doping: A DFT Investigation of Electronic Structure, AIM, NMR, NQR and NBO Analysis

Journal of Cluster Science, (29): 101-110. 2018. 10.1007/s10876-017-1310-1

Ghiasuddin; Akram, M.; Adeel, M.; Khalid, M.; Tahir, M. N.; Khan, M. U.; Asghar, M. A.; Ullah, M. A.; Iqbal, M.

A combined experimental and computational study of 3-bromo-5-(2,5-difluorophenyl) pyridine and 3,5-bis(naphthalen-1-yl)pyridine: Insight into the synthesis, spectroscopic, single crystal XRD, electronic, nonlinear optical and biological properties

Journal of Molecular Structure, (1160): 129-141. 2018. 10.1016/j.molstruc.2018.01.100

Gholipour, A.

Mutual interplay between pnicogen-pi and tetrel bond in PF<sub>3</sub> perpendicular to X-Pyr center dot center dot SiH<sub>3</sub>CN complexes: NMR, SAPT, AIM, NBO, and MEP analysis

Structural Chemistry, (29): 1255-1263. 2018. 10.1007/s11224-018-1106-4

Gholivand, K.; Kahnouji, M.; Maghsoud, Y.; Masumian, E.; Hosseini, M.

A theoretical study on the coordination behavior of some phosphoryl, carbonyl and sulfoxide derivatives in lanthanide complexation

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3865-7

Ghorai, P.; Brandao, P.; Bauza, A.; Frontera, A.; Saha, A.

Anion-reliant structural versatility of novel cadmium(II) complexes: Synthesis, crystal structures, photoluminescence properties and exploration of unusual O center dot center dot center dot S chalcogen bonding involving thiocyanate coligand

Inorganica Chimica Acta, (469): 189-196. 2018. 10.1016/j.ica.2017.09.005

Ghorai, S.; Jemmis, E. D.

B-B Coupling and B-B Catenation: Computational Study of the Structure and Reactions of Metal-Bis(borylene) Complexes

Chemistry-a European Journal, (24): 17844-17851. 2018. 10.1002/chem.201804599

Ghosh, K.; Harms, K.; Bauza, A.; Frontera, A.; Chattopadhyay, S.

Heteronuclear cobalt(III)/sodium complexes with salen type compartmental Schiff base ligands: methylene spacer regulated variation in nuclearity

Dalton Transactions, (47): 331-347. 2018. 10.1039/c7dt03929h

Ghosh, S.; Banerjee, P.; Nandi, P. K.

Heterolytic N-H bond activation of ammonia by dinuclear {M(mu-OMe)}<sub>2</sub> complexes (M = Sc - V and Mn - Ni): A theoretical investigation

Computational and Theoretical Chemistry, (1145): 44-53. 2018. 10.1016/j.comptc.2018.11.002

Giacomazzi, L.; Martin-Samos, L.; Alessi, A.; Valant, M.; Gunturu, K. C.; Boukenter, A.; Ouerdane, Y.; Girard, S.; Richard, N.

Optical absorption spectra of P defects in vitreous silica

Optical Materials Express, (8): 385-400. 2018. 10.1364/ome.8.000385

Giricheva, N. I.; Kurbatova, M. S.; Tyunina, E. Y.; Barannikov, V. P.

A Quantum Chemical Simulation of the Interaction Between Leucine and the Dimer of Sodium Dodecyl Sulphate

Journal of Structural Chemistry, (59): 1768-1775. 2018. 10.1134/s0022476618080024

Gleiter, R.; Haberhauer, G.; Werz, D. B.; Rominger, F.; Bleiholder, C.

From Noncovalent Chalcogen-Chalcogen Interactions to Supramolecular Aggregates: Experiments and Calculations

Chemical Reviews, (118): 2010-2041. 2018. 10.1021/acs.chemrev.7b00449

Glendening, E. D.; Weinhold, F.

Efficient evaluation of poly-electron populations in natural bond orbital analysis

Chemical Physics Letters, (711): 23-26. 2018. 10.1016/j.cplett.2018.09.013

Glendening, E. D.; Weinhold, F.

Natural resonance theory of chemical reactivity, with illustrative application to intramolecular Claisen rearrangement

Tetrahedron, (74): 4799-4804. 2018. 10.1016/j.tet.2018.07.054

- Goettel, J. T.; Mercier, H. P. A.; Schrobilgen, G. J.  
XeO<sub>3</sub> adducts of pyridine, 4-dimethylaminopyridine, and their pyridinium salts  
*Journal of Fluorine Chemistry*, (211): 60-69. 2018. 10.1016/j.jfluchem.2018.03.004
- Gokce, H.; Dede, B.; Bahceli, S.  
Structural, spectroscopic and quantum chemical studies on copper(II) complex of 4-ethoxy-2-methyl-5-(4-morpholinyl)-3(2H)-pyridazinone  
*Journal of Molecular Structure*, (1171): 471-480. 2018. 10.1016/j.molstruc.2018.06.034
- Gokce, H.; Sert, Y.; Ozturk, N.; Abdel-Aziz, A. A. M.; El-Azab, A. S.; Al-Obaid, A. M.  
Experimental and theoretical investigations on structural, spectroscopic, electronic and thermodynamic properties of (adamantan-1-yl)(phenylsulfanyl)methanone  
*Journal of Molecular Structure*, (1173): 596-607. 2018. 10.1016/j.molstruc.2018.07.031
- Goktas, M.; Bolli, C.; Berg, E. J.; Novak, P.; Pollok, K.; Langenhorst, F.; Roeder, M. V.; Lenchuk, O.; Mollenhauer, D.; Adelhelm, P.  
Graphite as Cointercalation Electrode for Sodium-Ion Batteries: Electrode Dynamics and the Missing Solid Electrolyte Interphase (SEI)  
*Advanced Energy Materials*, (8) 2018. 10.1002/aenm.201702724
- Gomes, G. D.; Loginova, Y.; Vatsadze, S. Z.; Alabugin, I. V.  
Isonitriles as Stereoelectronic Chameleons: The Donor-Acceptor Dichotomy in Radical Additions  
*Journal of the American Chemical Society*, (140): 14272-14288. 2018. 10.1021/jacs.8b08513
- Gong, S. D.; Chen, G. T.; Li, Q. S.; Luo, Q.; Xie, Y. M.; King, R. B.  
Cyclopentadienyliron boronyl carbonyls as isoelectronic analogues of cyclopentadienylmanganese carbonyls except for boronyl ligand coupling reactions  
*Inorganica Chimica Acta*, (475): 8-17. 2018. 10.1016/j.ica.2017.07.063
- Gong, X. L.; Zhu, L. Y.; Zhao, J. F.; Cui, G. M.; Lu, X. M.; Xie, Y. M.; King, R. B.  
Tetranuclear iron carbonyl complexes with a central tin atom: relationship to iron carbonyl carbides  
*New Journal of Chemistry*, (42): 10898-10905. 2018. 10.1039/c8nj01434e
- Gonzalez-Navarrete, P.; Andres, J.; Calatayud, M.  
Can Supported Reduced Vanadium Oxides form H<sub>2</sub> from CH<sub>3</sub>OH? A Computational Gas-Phase Mechanistic Study  
*Journal of Physical Chemistry A*, (122): 1104-1113. 2018. 10.1021/acs.jpca.7b11264
- Googheri, M. S.; Googheri, M. S. S.; Araghi, S. H.  
Configurational effect on ion-pair interaction energies and intermolecular potential energy functions in imidazolium-based ionic liquids: A theoretical study  
*Journal of Molecular Liquids*, (263): 158-173. 2018. 10.1016/j.molliq.2018.04.105

Gordeev, E. G.; Eremin, D. B.; Chernyshev, V. M.; Ananikov, V. P.  
Influence of R-NHC Coupling on the Outcome of R-X Oxidative Addition to Pd/NHC Complexes (R = Me, Ph, Vinyl, Ethynyl)  
*Organometallics*, (37): 787-796. 2018. 10.1021/acs.organomet.7b00669

Goud, Z.; Ben Said, R.; Sanhoury, M. A.; Boughdiri, S.; Prakash, M.; Linguerri, R.; Hochlaf, M.  
Insights into the bonding between tributylphosphine chalcogenides and zinc(II)  
*Theoretical Chemistry Accounts*, (137) 2018. 10.1007/s00214-018-2245-9

Grabowski, S. J.  
Coordination of Be and Mg Centres by HCN Ligands - Be...N and Mg...N Interactions  
*Chemphyschem*, (19): 1830-1840. 2018. 10.1002/cphc.201800274

Grabowski, S. J.  
Hydrogen bonds and other interactions as a response to protect doublet/octet electron structure  
*Journal of Molecular Modeling*, (24) 2018. 10.1007/s00894-017-3569-4

Grabowski, S. J.  
Magnesium Bonds: From Divalent Mg Centres to Trigonal and Tetrahedral Coordination  
*Chemistryselect*, (3): 3147-3154. 2018. 10.1002/slct.201703137

Grabowski, S. J.  
Tetrel Bonds with  $\pi$ -Electrons Acting as Lewis BasesTheoretical Results and Experimental Evidences  
*Molecules*, (23) 2018. 10.3390/molecules23051183

Grabowski, S. J.  
Two faces of triel bonds in boron trihalide complexes  
*Journal of Computational Chemistry*, (39): 472-480. 2018. 10.1002/jcc.25056

Green, M. L.; Jean, P.; Heaven, M. C.  
Dative Bonding between Closed-Shell Atoms: The BeF<sup>-</sup> Anion  
*Journal of Physical Chemistry Letters*, (9): 1999-2002. 2018. 10.1021/acs.jpclett.8b00784

Greenacre, V. K.; Levason, W.; Reid, G.  
Trialkylstibine Complexes of Boron, Aluminum, Gallium, and Indium Trihalides: Synthesis, Properties, and Bonding  
*Organometallics*, (37): 2123-2135. 2018. 10.1021/acs.organomet.8b00265

Greisch, J. F.; Ballester-Caudet, A.; Kruppa, S. V.; Lei, Z.; Wang, Q. M.; Riehn, C.; Remacle, F.  
Gas-Phase Photoluminescence and Photodissociation of Silver-Capped Hexagold Clusters  
*Journal of Physical Chemistry A*, (122): 5799-5810. 2018. 10.1021/acs.jpca.8b01864

- Grenon, N.; Baumgartner, T.  
Exploration of Hypervalent Lewis Acid/Base Interactions in 2-(2'-Thiazolyl)-3-thienylphosphanes  
*Inorganic Chemistry*, (57): 1630-1644. 2018. 10.1021/acs.inorgchem.7b03008
- Gribanova, T. N.; Minyaev, R. M.; Minkin, V. I.  
Stabilization of boron clusters with classical fullerene structures by combined doping effect: a quantum chemical study  
*Structural Chemistry*, (29): 327-340. 2018. 10.1007/s11224-017-1031-y
- Gribanova, T. N.; Minyaev, R. M.; Minkin, V. I.; Boldyrev, A. I.  
Metalcarbonyl analogues of annelated cyclooctatetraene and cyclodecapentaene derivatives with a planar core cycle: a quantum chemical study  
*Physical Chemistry Chemical Physics*, (20): 27830-27837. 2018. 10.1039/c8cp05444d
- Grimes, T. S.; Heathman, C. R.; Jansone-Popova, S.; Ivanov, A. S.; Roy, S.; Bryantsev, V. S.; Zalupski, P. R.  
Influence of a Heterocyclic Nitrogen-Donor Group on the Coordination of Trivalent Actinides and Lanthanides by Aminopolycarboxylate Complexants  
*Inorganic Chemistry*, (57): 1373-1385. 2018. 10.1021/acs.inorgchem.7b02792
- Grissom, T. G.; Sharp, C. H.; Usov, P. M.; Troya, D.; Morris, A. J.; Morris, J. R.  
Benzene, Toluene, and Xylene Transport through UiO-66: Diffusion Rates, Energetics, and the Role of Hydrogen Bonding  
*Journal of Physical Chemistry C*, (122): 16060-16069. 2018. 10.1021/acs.jpcc.8b03356
- Grune, E.; Johann, T.; Appold, M.; Wahlen, C.; Blankenburg, J.; Leibig, D.; Muller, A. H. E.; Gallei, M.; Frey, H.  
One-Step Block Copolymer Synthesis versus Sequential Monomer Addition: A Fundamental Study Reveals That One Methyl Group Makes a Difference  
*Macromolecules*, (51): 3527-3537. 2018. 10.1021/acs.macromol.8b00404
- Grunwald, A.; Munz, D.  
How to tame a palladium terminal imido  
*Journal of Organometallic Chemistry*, (864): 26-36. 2018. 10.1016/j.jorgchem.2017.12.034
- Gruzdev, M. S.; Krestyaninov, M. A.; Krylov, E. N.; Shmukler, L. E.; Safonova, L. P.  
Possibility of Protic Ionic Liquids Formation From Triethanolamine with Sulfonamides  
*Journal of Physical Chemistry B*, (122): 6586-6594. 2018. 10.1021/acs.jpcb.8b02981
- Guddorf, B. J.; Hepp, A.; Lips, F.  
Efficient Synthesis of a NHC-Coordinated Trisilacyclopropylidene and Its Coordination Behavior  
*Chemistry-a European Journal*, (24): 10334-10338. 2018. 10.1002/chem.201802625
- Guelai, A.; Brahim, H.; Guendouzi, A.; Boumediene, M.; Brahim, S.

Structure, electronic properties, and NBO and TD-DFT analyses of nickel(II), zinc(II), and palladium(II) complexes based on Schiff-base ligands

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3839-9

Guerra, R. J.; Lezama, J.; Cordova-Sintjago, T.; Chuchani, G.

Theoretical calculations of homogeneous catalysis in the gas phase: elimination kinetics of 2,2-dimethoxypropane in the presence of HCl, F<sub>3</sub>CCOOH and CH<sub>3</sub>COOH

Molecular Physics, (116): 1118-1126. 2018. 10.1080/00268976.2017.1406621

Gultekin, Z.; Demircioglu, Z.; Frey, W.; Buyukgungor, O.

XRD, Spectroscopic characterization (FT-IR, UV-Vis), Hirshfeld surface analysis and chemical activity of (E)-benzyl 2-((2S,3S,4R)-2,3,4-tris(benzyloxy)hex-5-enylidene) hydrazinecarboxylate

Journal of Molecular Structure, (1171): 375-387. 2018. 10.1016/j.molstruc.2018.05.076

Gumustas, S.; Balcan, M.; Kinal, A.

Computational determination of ring opening polymerization reaction mechanism of alpha-angelica lactone

Computational and Theoretical Chemistry, (1142): 1-8. 2018. 10.1016/j.comptc.2018.08.022

Guo, J. C.; Feng, L. Y.; Dong, C.; Zhai, H. J.

Planar Pentacoordinate versus Tetracoordinate Carbons in Ternary CBe4Li4 and CBe4Li42-Clusters

Journal of Physical Chemistry A, (122): 8370-8376. 2018. 10.1021/acs.jpca.8b08573

Guo, J. C.; Feng, L. Y.; Zhai, H. J.

Ternary CBe4Au4 cluster: a 16-electron system with quasi-planar tetracoordinate carbon

Physical Chemistry Chemical Physics, (20): 6299-6306. 2018. 10.1039/c7cp08420j

Guo, J. C.; Feng, L. Y.; Zhang, X. Y.

Low-dimensional nanocomplexes based on planar tetracoordinate Si/Ge: Nanoribbons

X<sub>n</sub>NiC<sub>2n+2</sub>Cl<sub>2n+2</sub> (X = Si, Ge) and nanotubes Si<sub>n</sub>Ni<sub>2n</sub>Cl<sub>2n</sub>

Computational and Theoretical Chemistry, (1128): 24-30. 2018. 10.1016/j.comptc.2018.02.009

Guo, J. C.; Feng, L. Y.; Zhang, X. Y.

Planar tetracoordinate carbon CNi4H4 cluster and its nanoribbon complexes

(C<sub>n</sub>Ni<sub>4</sub>H<sub>2</sub>)<sub>(n)</sub>(C<sub>4</sub>H<sub>6</sub>)<sub>(n+1)</sub> (n=1-4) stabilized using aromatic butadiene ligands

Computational and Theoretical Chemistry, (1125): 95-102. 2018. 10.1016/j.comptc.2018.01.011

Guo, J. C.; Feng, L. Y.; Zhang, X. Y.; Zhai, H. J.

Star-Like CBe5Au5+ Cluster: Planar Pentacoordinate Carbon, Superalkali Cation, and Multifold ( $\pi$  and sigma) Aromaticity

Journal of Physical Chemistry A, (122): 1138-1145. 2018. 10.1021/acs.jpca.7b11789

Guo, J. D.; Lu, Y.; Zhao, R. H.; Liu, Z. Y.; Menberu, W.; Wang, Z. X.

Strong Preference of the Redox-Neutral Mechanism over the Redox Mechanism for the Ti-IV Catalysis Involved in the Carboamination of Alkyne with Alkene and Diazene  
Chemistry-a European Journal, (24): 7010-7025. 2018. 10.1002/chem.201800339

Guo, L. H.; Zhang, H. R.; Tian, M.; Tian, Z. Z.; Xu, Y. J.; Yang, Y. L.; Peng, H. W.; Liu, P.; Liu, Z.  
Electronic effects on reactivity and anticancer activity by half-sandwich N,N-chelated iridium(III) complexes  
New Journal of Chemistry, (42): 16183-16192. 2018. 10.1039/c8nj03360a

Guo, M. G.; Cao, Z. L.; Wang, Z. F.; Wang, F.  
Properties of closed-shell superheavy element hydrides and halides using coupled-cluster method and density functional theory with spin-orbit coupling  
Journal of Chemical Physics, (148) 2018. 10.1063/1.5011648

Guo, X. J.; Li, C.; Hu, J. T.; Ma, H. J.; Qian, H. L.  
A density functional theory study on the interaction between UO<sub>2</sub><sup>2+</sup> and the carbamoylphosphoramidic acid ligand for uranium extraction from seawater  
Nuclear Science and Techniques, (29) 2018. 10.1007/s41365-018-0422-0

Gurav, N. D.; Gejji, S. P.; Pathak, R. K.  
Electronic Stark effect for a single molecule: Theoretical UV response  
Computational and Theoretical Chemistry, (1138): 23-38. 2018. 10.1016/j.comptc.2018.05.018

Gurusinghe, R. M.; Tubergen, M. J.  
Microwave spectra of 2-phenylethyl methyl ether and 2-phenylethyl methyl ether-argon:  
Conformation-dependent tunneling and complexation  
Journal of Molecular Spectroscopy, (346): 13-18. 2018. 10.1016/j.jms.2017.12.012

Gutsev, G. L.; Belay, K. G.; Gutsev, L. G.; Ramachandran, B. R.; Jena, P.  
Effect of hydrogenation on the structure and magnetic properties of an iron oxide cluster  
Physical Chemistry Chemical Physics, (20): 4546-4553. 2018. 10.1039/c7cp08224j

Gutsev, G. L.; Bozhenko, K. V.; Gutsev, L. G.; Utenshev, A. N.; Aldoshin, S. M.  
Dependence of Properties and Exchange Coupling Constants on the Charge in the Mn<sub>2</sub>O<sub>n</sub> and Fe<sub>2</sub>O<sub>n</sub> Series  
Journal of Physical Chemistry A, (122): 5644-5655. 2018. 10.1021/acs.jpca.8b03496

Gutsev, L. G.; Gutsev, G. L.; Jena, P.  
Collective Superexchange and Exchange Coupling Constants in the Hydrogenated Iron Oxide Particle Fe<sub>8</sub>O<sub>12</sub>H<sub>8</sub>  
Journal of Physical Chemistry A, (122): 5043-5049. 2018. 10.1021/acs.jpca.8b03034

Gyton, M. R.; Leforestier, B.; Chaplin, A. B.

Rhodium(III) and Iridium(III) Complexes of a NHC-Based Macrocycle: Persistent Weak Agostic Interactions and Reactions with Dihydrogen

Organometallics, (37): 3963-3971. 2018. 10.1021/acs.organomet.8b00595

Hadji, D.; Brahim, H.

Structural, optical and nonlinear optical properties and TD-DFT analysis of heteroleptic bis-cyclometalated iridium(III) complex containing 2-phenylpyridine and picolinate ligands

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2396-8

Haghdadi, M.; Alashti, M.; Bosra, H. G.

A theoretical investigation on the mechanism of cycloaddition reactions of fulvenes with tetrazine and diazacyclopentadienone derivatives

Structural Chemistry, (29): 1511-1523. 2018. 10.1007/s11224-018-1138-9

Haghdadi, M.; Nab, N.

A theoretical study on the regio- and stereoselectivity of 3+2 cycloaddition of 2-(trifluoroacetyl)vinyl ethyl ether to 2-arylidene-5-oxopyrazolidin-2-iun-1-ides

Journal of the Serbian Chemical Society, (83): 285-303. 2018. 10.2298/jsc170511099h

Hailu, Y. M.; Nguyen, M. T.; Jiang, J. C.

Effects of the terminal donor unit in dyes with D-D-pi-A architecture on the regeneration mechanism in DSSCs: a computational study

Physical Chemistry Chemical Physics, (20): 23564-23577. 2018. 10.1039/c8cp03821j

Haines, B. E.; Sarpong, R.; Musaev, D. G.

Generality and Strength of Transition Metal beta-Effects

Journal of the American Chemical Society, (140): 10612-10618. 2018. 10.1021/jacs.8b06817

Hakiri, R.; Ameur, I.; Abid, S.; Derbel, N.

Synthesis, X-ray structural, Hirshfeld surface analysis, FTIR, MEP and NBO analysis using DFT study of a 4-chlorobenzylammonium nitrate (C<sub>7</sub>ClH<sub>9</sub>N)(+)(NO<sub>3</sub>

Journal of Molecular Structure, (1164): 486-492. 2018. 10.1016/j.molstruc.2018.03.068

Halder, A.; Roy, R.; Bhattacharyya, D.; Mitra, A.

Consequences of Mg<sup>2+</sup> binding on the geometry and stability of RNA base pairs

Physical Chemistry Chemical Physics, (20): 21934-21948. 2018. 10.1039/c8cp03602k

Halim, S.

Theoretical Study and Experimental Analysis on 2-(1-Ethyl-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl)-2-oxoacetic Acid (3) Using the DFT Approach

Journal of Solution Chemistry, (47): 172-197. 2018. 10.1007/s10953-018-0713-4

Halim, S. A.; Adly, O. M. I.

DFT Calculations, Spectroscopic Studies, Biological Activity and Non Linear Optical Properties (NLO) of Novel Ternary Cu(II)-Chelates Derived from 5-Acetyl-4-hydroxy-2H-1,3-thiazinedione  
Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4435

Hallooman, D.; Rios-Gutierrez, M.; Rhyman, L.; Alswaidan, I. A.; Domingo, L. R.; Ramasami, P.  
DFT exploration of 3+2 cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl methacrylate  
RSC Advances, (8): 27406-27416. 2018. 10.1039/c8ra04703k

Hamza-Reguig, S.; Bentabed-Ababsa, G.; Domingo, L. R.; Rios-Gutierrez, M.; Philippot, S.; Fontanay, S.; Duval, R. E.; Ruchaud, S.; Bach, S.; Roisnel, T.; Mongin, F.  
A combined experimental and theoretical study of the thermal 3+2 cycloaddition of carbonyl ylides with activated alkenes  
Journal of Molecular Structure, (1157): 276-287. 2018. 10.1016/j.molstruc.2017.12.052

Hanft, A.; Lichtenberg, C.  
Aminotroponimimates: ligand-centred, reversible redox events under oxidative conditions in sodium and bismuth complexes  
Dalton Transactions, (47): 10578-10589. 2018. 10.1039/c8dt01019f

Hanft, A.; Lichtenberg, C.  
Rationalizing the Effect of Ligand Substitution Patterns on Coordination and Reactivity of Alkali Metal Aminotroponimimates  
Organometallics, (37): 1781-1787. 2018. 10.1021/acs.organomet.8b00208

Hao, A. Q.; Xu, B. Z.; Jia, J. F.  
An insight into the structures, stabilities and magnetic properties of Fe<sub>2</sub>Bn (n=1-10) clusters  
Materials Chemistry and Physics, (205): 1-8. 2018. 10.1016/j.matchemphys.2017.10.066

Haque, M. R.; Ghosh, S.; Rahman, M. M.; Siddiquee, T. A.; Nesterov, V. N.; Richmond, M. G.; Hogarth, G.; Kabir, S. E.  
Mixed-valence dimolybdenum complexes containing hard oxo and soft carbonyl ligands: synthesis, structure, and electrochemistry of Mo<sub>2</sub>(O)(CO)(2)(μ<sub>2</sub>-κ<sub>2</sub>S(CH<sub>2</sub>)<sub>n</sub>S)(2)(κ<sub>2</sub>-diphosphine)  
Dalton Transactions, (47): 10102-10112. 2018. 10.1039/c8dt02231c

Harada, T.  
Dinuclear Tricyclic Transition State Model for Carbonyl Addition of Organotitanium Reagents: DFT Study on the Activity and Enantioselectivity of BINOLate Titanium Catalysts  
Journal of Organic Chemistry, (83): 7825-7835. 2018. 10.1021/acs.joc.8b00712

Haraga, T.; Ouchi, K.; Sato, Y.; Hoshino, H.; Tanaka, R.; Fujihara, T.; Kurokawa, H.; Shibukawa, M.; Ishimori, K.; Kameo, Y.; Saito, S.

Safe and rapid development of capillary electrophoresis for ultratrace uranyl ions in radioactive samples by way of fluorescent probe selection for actinide ions from a chemical library  
Analytica Chimica Acta, (1032): 188-196. 2018. 10.1016/j.aca.2018.05.077

Harchani, A.; Haddad, A.  
New diphosphopentamolybdate (VI) ( $C_6H_{14}N(4)(NH_4)(2)$ ) $P_2Mo_5O_{23}$  center dot  $H_2O$  synthesis, crystal structure, experimental and theoretical studies  
Bulletin of Materials Science, (41) 2018. 10.1007/s12034-018-1561-y

Harinath, A.; Bhattacharjee, J.; Gorantla, K. R.; Mallik, B. S.; Panda, T. K.  
Hydroboration, Cyanosilylation, and Sequential Cyanosilylation and Hydroboration of Carbonyl Compounds in the Presence of a Ti-IV Amido Complex as an Efficient Catalyst  
European Journal of Organic Chemistry: 3180-3192. 2018. 10.1002/ejoc.201800547

Harrath, K.; Boughdiri, S.  
High catalytic activity of Ti-porphyrin for NO reduction by CO: a first-principles study  
Research on Chemical Intermediates, (44): 957-969. 2018. 10.1007/s11164-017-3146-6

Hasan, T.; Ghalib, R. M.; Mehdi, S. H.; Singh, P. K.; Kumar, A.; Misra, N.  
Vibrational Spectra, NBO and NLO Analyses, and A Molecular Docking Study of 3a,8a-Dihydroxy-2-Thioxo-1,3,3a,8a-Tetrahydroindeno 1,2-d Imidazol-8(2H) -One Using DFT  
Journal of Structural Chemistry, (59): 1078-1087. 2018. 10.1134/s0022476618050098

Hasanzade, Z.; Raissi, H.  
Density functional theory calculations. and molecular dynamics simulations of the adsorption of ellipticine anticancer drug on graphenc oxide surface in aqueous medium as well as under controlled pH conditions  
Journal of Molecular Liquids, (255): 269-278. 2018. 10.1016/j.molliq.2018.01.159

Hasegawa, E.; Nagakura, Y.; Izumiya, N.; Matsumoto, K.; Tanaka, T.; Miura, T.; Ikoma, T.; Iwamoto, H.; Wakamatsu, K.  
Visible Light and Hydroxynaphthylbenzimidazoline Promoted Transition-Metal-Catalyst-Free Desulfonylation of N-Sulfonylamides and N-Sulfonylaminines  
Journal of Organic Chemistry, (83): 10813-10825. 2018. 10.1021/acs.joc.8b01536

Hashemzadeh, H.; Raissi, H.  
Covalent organic framework as smart and high efficient carrier for anticancer drug delivery: a DFT calculations and molecular dynamics simulation study  
Journal of Physics D-Applied Physics, (51) 2018. 10.1088/1361-6463/aad3e8

Haslak, Z. P.; Bozkurt, E.; Dutagaci, B.; De Proft, F.; Aviyente, V.; De Vleeschouwer, F.  
A DFT approach to discriminate the antagonist and partial agonist activity of ligands binding to the NMDA receptor  
Molecular Physics, (116): 323-337. 2018. 10.1080/00268976.2017.1384579

Hayashi, S.; Tsubomoto, Y.; Nakanishi, W.

Behavior of the E-E' Bonds (E, E' = S and Se) in Glutathione Disulfide and Derivatives Elucidated by Quantum Chemical Calculations with the Quantum Theory of Atoms-In-Molecules Approach

Molecules, (23) 2018. 10.3390/molecules23020443

He, J. Y.; Han, H. S.; Zhang, C. Y.; Hu, Y. H.; Yuan, D. D.; Tian, M. J.; Chen, D. X.; Sun, W.

New Insights into the Configurations of Lead(II)-Benzohydroxamic Acid Coordination Compounds in Aqueous Solution: A Combined Experimental and Computational Study

Minerals, (8) 2018. 10.3390/min8090368

He, Y. Q.; Teng, J. W.; Tian, C.; Maxim, B.; Hu, Q. S.; Nie, W. L.

Reductive Amination by One Pot Reaction of Aldehydes and Alkoxyamines Catalyzed by B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>

Acta Chimica Sinica, (76): 774-778. 2018. 10.6023/a18070281

He, Z. L.; Feng, G.; Yang, B.; Yang, L. J.; Liu, C. W.; Xu, H. G.; Xu, X. L.; Zheng, W. J.; Gao, Y. Q.

Molecular dynamics simulation, ab initio calculation, and size-selected anion photoelectron spectroscopy study of initial hydration processes of calcium chloride

Journal of Chemical Physics, (148) 2018. 10.1063/1.5024279

Heathman, C. R.; Grimes, T. S.; Jansone-Popova, S.; Ivanov, A. S.; Bryantsev, V. S.; Zalupska, P. R.

Synthesis and characterization of a novel aminopolycarboxylate complexant for efficient trivalent f-element differentiation: N-butyl-2-acetamide-diethylenetriamine-N, N', N'', N'''-tetraacetic acid

Dalton Transactions, (47): 1092-1105. 2018. 10.1039/c7dt04104g

Heidar-Zadeh, F.; Ayers, P. W.

Generalized Hirshfeld Partitioning with Oriented and Promoted Proatoms

Acta Physico-Chimica Sinica, (34): 514-518. 2018. 10.3866/pku.Whxb201710101

Heidar-Zadeh, F.; Ayers, P. W.; Verstraelen, T.; Vinogradov, I.; Vohringer-Martinez, E.; Bultinck, P.

Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes

Journal of Physical Chemistry A, (122): 4219-4245. 2018. 10.1021/acs.jpca.7b08966

Heller, B. S. J.; Kolbeck, C.; Niedermaier, I.; Dommer, S.; Schatz, J.; Hunt, P.; Maier, F.; Steinruck, H. P.

Surface Enrichment in Equimolar Mixtures of Non-Functionalized and Functionalized Imidazolium-Based Ionic Liquids

Chemphyschem, (19): 1733-1745. 2018. 10.1002/cphc.201800216

Henoch, J.; Auch, A.; Diab, F.; Eichele, K.; Schubert, H.; Sirsch, P.; Block, T.; Pottgen, R.; Wesemann, L.

Cyclic Distannene or Bis(stannylene) with a Ferrocenyl Backbone: Synthesis, Structure, and Coordination Chemistry

Inorganic Chemistry, (57): 4135-4145. 2018. 10.1021/acs.inorgchem.8b00317

Hepp, A.; Labbow, R.; Reiss, F.; Schulz, A.; Villinger, A.

Carba-closo-dodecaborates - Synthesis, Structure, and Energetics

European Journal of Inorganic Chemistry: 2905-2914. 2018. 10.1002/ejic.201800219

Herbig, M.; Bohme, U.; Kroke, E.

Insertion of CO<sub>2</sub> and related heteroallenes into the Si-N-bond of methyl (N-morpholino) silanes

Inorganica Chimica Acta, (473): 20-28. 2018. 10.1016/j.ica.2017.12.020

Hesabi, M.; Behjatmanesh-Ardakani, R.

Investigation of carboxylation of carbon nanotube in the adsorption of anti-cancer drug: A theoretical approach

Applied Surface Science, (427): 112-125. 2018. 10.1016/j.apsusc.2017.08.044

Hiberty, P. C.; Braida, B.

Pleading for a Dual Molecular-Orbital/Valence-Bond Culture

Angewandte Chemie-International Edition, (57): 5994-6002. 2018. 10.1002/anie.201710094

Hidayat, Y.; Armunanto, R.; Pranowo, H. D.

Investigation of rubidium(I) ion solvation in liquid ammonia using QMCF-MD simulation and NBO analysis of first solvation shell structure

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3668-x

Hidayat, Y.; Pranowo, H. D.; Armunanto, R.

Revisiting structure and dynamics of preferential solvation of K(I) ion in aqueous ammonia using QMCF-MD simulation

Chemical Physics Letters, (699): 234-240. 2018. 10.1016/j.cplett.2018.03.067

Hijas, K. M.; Kumar, S. M.; Byrappa, K.; Geethakrishnan, T.; Jeyaram, S.; Nagalakshmi, R.

Spectroscopic investigations using density functional theory on 2-methoxy-4(phenyliminomethyl)phenol: A non linear optical material

Journal of Molecular Structure, (1155): 249-259. 2018. 10.1016/j.molstruc.2017.11.001

Himmelbauer, D.; Mastalir, M.; Stoger, B.; Veiros, L. F.; Kirchner, K.

Synthesis and Reactivity of Group Six Metal PCP Pincer Complexes: Reversible CO Addition Across the Metal-C-aryl Bond

Organometallics, (37): 3631-3638. 2018. 10.1021/acs.organomet.8b00447

Himmelbauer, D.; Mastalir, M.; Stoger, B.; Veiros, L. F.; Pignitter, M.; Somoza, V.; Kirchner, K.

Iron PCP Pincer Complexes in Three Oxidation States: Reversible Ligand Protonation To Afford an Fe(0) Complex with an Agostic C-H Arene Bond

Inorganic Chemistry, (57): 7925-7931. 2018. 10.1021/acs.inorgchem.8b01018

Himmelbauer, D.; Stoger, B.; Veiros, L. F.; Kirchner, K.

Reversible Ligand Protonation of a Mn(I) PCP Pincer Complex To Afford a Complex with an eta(2)-C-aryl-H Agostic Bond

Organometallics, (37): 3475-3479. 2018. 10.1021/acs.organomet.8b00193

Hiremath, S. M.; Suvitha, A.; Patil, N. R.; Hiremath, C. S.; Khemalapure, S. S.; Pattanayak, S. K.; Negalurmath, V. S.; Obelannavar, K.

Molecular structure, vibrational spectra, NMR, UV, NBO, NLO, HOMO-LUMO and molecular docking of 2-(4, 6-dimethyl-1-1-benzofuran-3-yl) acetic acid (2DBAA): Experimental and theoretical approach

Journal of Molecular Structure, (1171): 362-374. 2018. 10.1016/j.molstruc.2018.05.109

Hiremath, S. M.; Suvitha, A.; Patil, N. R.; Hiremath, C. S.; Khemalapure, S. S.; Pattanayak, S. K.; Negalurmath, V. S.; Obelannavar, K.; Armakovic, S. J.; Arrnakovic, S.

Synthesis of 5-(5-methyl-benzofuran-3-ylmethyl)-3H-1,3,4 oxadiazole-2-thione and investigation of its spectroscopic, reactivity, optoelectronic and drug likeness properties by combined computational and experimental approach

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (205): 95-110. 2018. 10.1016/j.saa.2018.07.003

Hirshberg, B.; Gerber, R. B.; Krylov, A. I.

Autocorrelation of electronic wave-functions: a new approach for describing the evolution of electronic structure in the course of dynamics

Molecular Physics, (116): 2512-2523. 2018. 10.1080/00268976.2018.1464675

Hirshberg, B.; Molina, E. A. R.; Gotz, A. W.; Hammerich, A. D.; Nathanson, G. M.; Bertram, T. H.; Johnson, M. A.; Gerber, R. B.

N<sub>2</sub>O<sub>5</sub> at water surfaces: binding forces, charge separation, energy accommodation and atmospheric implications

Physical Chemistry Chemical Physics, (20): 17961-17976. 2018. 10.1039/c8cp03022g

Hofer, T. S.; Hunenberger, P. H.

Absolute proton hydration free energy, surface potential of water, and redox potential of the hydrogen electrode from first principles: QM/MM MD free-energy simulations of sodium and potassium hydration

Journal of Chemical Physics, (148) 2018. 10.1063/1.5000799

Hoffmann, G.; Tognetti, V.; Joubert, L.

Can molecular and atomic descriptors predict the electrophilicity of Michael acceptors?

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3802-9

Hollingsworth, R. L.; Beattie, J. W.; Grass, A.; Martin, P. D.; Groysman, S.; Lord, R. L.

Reactions of dicobalt octacarbonyl with dinucleating and mononucleating bis(imino)pyridine ligands

Dalton Transactions, (47): 15353-15363. 2018. 10.1039/c8dt03405b

Holzmann, N.; Bernasconi, L.; Bisby, R. H.; Parker, A. W.

Influence of charge transfer on the isomerisation of stilbene derivatives for application in cancer therapy

Physical Chemistry Chemical Physics, (20): 27778-27790. 2018. 10.1039/c8cp05375h

Hoobler, P. R.; Turney, J. M.; Agarwal, J.; Schaefer, H. F.

Fundamental Vibrational Analyses of the HCN Monomer, Dimer and Associated Isotopologues  
Chemphyschem, (19): 3257-3265. 2018. 10.1002/cphc.201800728

Hosna, S.; Janzen, D. E.; Mary, Y. S.; Resmi, K. S.; Thomas, R.; Mohamed, R.; Wajda, S.

Molecular structure, spectroscopic, dielectric and thermal study, nonlinear optical properties, natural bond orbital, HOMO-LUMO and molecular docking analysis of (C<sub>6</sub>Cl<sub>2</sub>O<sub>4</sub>) (C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>F)<sub>(2)</sub>center dot 2H<sub>(2)</sub>O

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (204): 328-339. 2018.  
10.1016/j.saa.2018.06.062

Hossain, M.; Thomas, R.; Mary, Y. S.; Resmi, K. S.; Armakovic, S.; Armakovic, S. J.; Nanda, A. K.; Vijayakumar, G.; Van Alsenoy, C.

Understanding reactivity of two newly synthesized imidazole derivatives by spectroscopic characterization and computational study

Journal of Molecular Structure, (1158): 176-196. 2018. 10.1016/j.molstruc.2018.01.029

Hosseini, S. M.; Zabardasti, A.

M center dot center dot center dot pi-conjugated complexes: simple materials with dramatic NLO features (M = Li, Na, K, and pi = butadiene, cyclobutadiene, hexatriene, benzene)

Structural Chemistry, (29): 415-422. 2018. 10.1007/s11224-017-1038-4

Hosseinian, A.; Nezhad, P. D. K.; Vessally, E.; Nejati, K.

Insight into electronic and structural properties of nLi@() nanotubules: a computational study  
Journal of Chemical Sciences, (130) 2018. 10.1007/s12039-018-1536-y

Hosseinian, A.; Vessally, E.; Babazadeh, M.; Edjlali, L.; Es'haghi, M.

On lithium doping in two stable nano-flakes of the B-24: The double-ring versus the quasiplanar configuration

Journal of Molecular Graphics & Modelling, (79): 213-222. 2018. 10.1016/j.jmgm.2017.11.012

Hosseini-Yazdi, S. A.; Samadzadeh-Aghdam, P.; Ghadari, R.

Synthesis and experimental/theoretical evaluations on redox potentials and electronic absorption spectra for copper symmetric bis (thiosemicarbazone) complexes

Polyhedron, (151): 221-232. 2018. 10.1016/j.poly.2018.05.034

Hou, H. Y.; Jiao, B. J.; Li, Q. Z.; Lin, X. L.; Liu, M.; Shi, H. J.; Wang, L.; Liu, S. T.

Physicochemical properties, NMR, Ab initio calculations and the molecular interactions in a binary mixture of N-methylimidazole and water

Journal of Molecular Liquids, (257): 100-111. 2018. 10.1016/j.molliq.2018.02.098

Hou, H. Y.; Jiao, B. J.; Li, Q. Z.; Lin, X. L.; Liu, S. T.

Physicochemical Properties, H-1-NMR, Ab Initio Calculations and Molecular Interaction in Binary Mixtures of N-methylimidazole with Methanol

Journal of Solution Chemistry, (47): 1875-1901. 2018. 10.1007/s10953-018-0824-y

Hou, J. H.; Liu, Y. J.; Zhang, X.; Duan, Q.; Jiang, D. Y.; Qin, J. M.; Zhao, R. Q.

Electric-field-induced nonlinear optical switches of all-metal spherical aromatic molecules with infrared transparency: a theoretical study

New Journal of Chemistry, (42): 1031-1036. 2018. 10.1039/c7nj03878j

Hou, J. H.; Wu, D.; Liu, J. Y.; Li, S. Y.; Yu, D.; Li, Y.

The effect of hydration on the electronic structure and stability of the superalkali cation Li-3(+)

Physical Chemistry Chemical Physics, (20): 15174-15182. 2018. 10.1039/c8cp00862k

Hou, S. L.; Qureshi, A. H.; Wei, Z. X.

Atomic Charges in Highly Ionic Diatomic Molecules

ACS Omega, (3): 17180-17187. 2018. 10.1021/acsomega.8b02370

Hou, X. F.; Fu, F.; Chang, Q.; Zhang, W. L.

DFT Study on the Germanium Ion Activated C-H Bond in Methane

Chinese Journal of Structural Chemistry, (37): 1533-1540. 2018. 10.14102/j.cnki.0254-5861.2011-1988

Hou, X. Y.; Wang, X.; Tang, L.; Wang, J. J.; Hou, X. F.; Kang, W. W.; Liu, X. L.

Synthesis, Structure, and Properties of { Mn(ADA)(Phen) center dot(H2O)(2)}(n) Constructed from Azobenzene-4,4'-dicarboxylic Acid and 1,10-Phenanthroline

Chinese Journal of Structural Chemistry, (37): 1125-1132. 2018. 10.14102/j.cnki.0254-5861.2011-1918

Hu, B.; Yi, Y.; Zhou, L.; Shen, A.; Liang, C.; Yang, L. J.; Roszak, S.

Experimental and DFT studies of PM2.5 removal by chemical agglomeration

Fuel, (212): 27-33. 2018. 10.1016/j.fuel.2017.09.121

Hu, J. Q.; Chen, L. T.; Shi, M. Q.; Zhang, C.

A quantum chemistry study for 1-ethyl-3-Methylimidazolium ion liquids with aprotic heterocyclic anions applied to carbon dioxide absorption

Fluid Phase Equilibria, (459): 208-218. 2018. 10.1016/j.fluid.2017.12.016

Hu, S. X.; Chen, M. Y.; Ao, B. Y.

Theoretical studies on the oxidation states and electronic structures of actinide-borides: AnB(12)  
(An = Th-Cm) clusters

Physical Chemistry Chemical Physics, (20): 23856-23863. 2018. 10.1039/c8cp02561d

Hu, S. X.; Liu, H. T.; Liu, J. J.; Zhang, P.; Ao, B. Y.

Electronic Structure and Chemical Bonding of AmO<sub>2</sub>(H<sub>2</sub>O)(n) (2+/1+)  
ACS Omega, (3): 13902-13912. 2018. 10.1021/acsomega.8b01324

Hu, S. X.; Liu, J. J.; Gibson, J. K.; Li, J.

Periodic Trends in Actinyl Thio-Crown Ether Complexes  
Inorganic Chemistry, (57): 2899-2907. 2018. 10.1021/acs.inorgchem.7b03277

Huang, C.; Lv, H. B.; Zuo, C.; Yuan, Z. W.; Zheng, W. F.; Yan, T. H.

Selective extraction of plutonium(IV) over uranium(VI), americium(III), europium(III) and zirconium(IV) with bidentate O-phenoxydiamide ligands: experimental and theoretical study  
Journal of Radioanalytical and Nuclear Chemistry, (317): 103-110. 2018. 10.1007/s10967-018-5836-y

Huang, F.; Wang, Q.; Guo, J. D.; Wen, M. W.; Wang, Z. X.

Computational mechanistic study of Ru-catalyzed CO<sub>2</sub> reduction by pinacolborane revealing the sigma-pi coupling mechanism for CO<sub>2</sub> decarbonylation  
Dalton Transactions, (47): 4804-4819. 2018. 10.1039/c8dt00081f

Huang, J. G.; Wang, Y. F.; Zhou, G. P.; Li, J.; Li, Z. R.

Theoretical insights into the magneto-structural correlation: Comparison between series of copper(I) and silver(I) metal complexes with nitronyl nitroxide radicals  
Computational and Theoretical Chemistry, (1141): 53-65. 2018. 10.1016/j.comptc.2018.08.008

Huang, M. J.; Feng, S. T.; Zhang, W. X.; Giordano, L.; Chen, M.; Amanchukwu, C. V.; Anandakathir, R.; Shao-Horn, Y.; Johnson, J. A.

Fluorinated Aryl Sulfonimide Tagged (FAST) salts: modular synthesis and structure-property relationships for battery applications  
Energy & Environmental Science, (11): 1326-1334. 2018. 10.1039/c7ee03509h

Huang, P. W.; Wang, C. Z.; Wu, Q. Y.; Lan, J. H.; Song, G.; Chai, Z. F.; Shi, W. Q.

Theoretical studies on the synergistic extraction of Am<sup>3+</sup> and Eu<sup>3+</sup> with CMPO-HDEHP and CMPO-HEH EHP systems

Dalton Transactions, (47): 5474-5482. 2018. 10.1039/c8dt00134k

Huang, P. W.; Wang, C. Z.; Wu, Q. Y.; Lan, J. H.; Song, G.; Chai, Z. F.; Shi, W. Q.

Understanding Am<sup>3+</sup>/Cm<sup>3+</sup> separation with H(4)TPAEN and its hydrophilic derivatives: a quantum chemical study

Physical Chemistry Chemical Physics, (20): 14031-14039. 2018. 10.1039/c7cp08441b

Huang, T. F.; Wang, Q.; Yu, W. J.; Wang, X. F.; Andrews, L.  
OMS, OM(eta(2)-SO), and OM(eta(2)-SO)(eta(2)-O2S) Molecules (M = Ce, Th) with Chiral  
Structure: Matrix Infrared Spectra and Theoretical Calculations  
Journal of Physical Chemistry A, (122): 5391-5400. 2018. 10.1021/acs.jpca.8b03731

Hussan, K. P. S.; Thayyil, M. S.; Rajan, V. K.; Muraleedharan, K.  
Experimental and density functional theory studies on benzalkonium ibuprofenate, a double  
active pharmaceutical ingredient  
Computational Biology and Chemistry, (72): 113-121. 2018.  
10.1016/j.compbiochem.2017.12.004

Ibeji, C. U.; Tolufashe, G. F.; Ntombela, T.; Govender, T.; Maguire, G. E. M.; Lamichhane, G.; Kruger, H. G.; Honarpourvar, B.  
The catalytic role of water in the binding site of L,D-transpeptidase 2 within acylation  
mechanism: A QM/MM (ONIOM) modelling  
Tuberculosis, (113): 222-230. 2018. 10.1016/j.tube.2018.10.005

Ibrahim, M.; Abbas, M.; Khalid, M.; Tahir, M. N.; Khan, M. U.; Hussain, A.; Ullah, A.; Hussain, A.  
Phytochemical, Crystal Structure, Spectroscopic, DFT Based Non Covalent Interactions and Non-  
Linear Optical Studies of Neurada procumbens  
Journal of the Chemical Society of Pakistan, (40): 749-760. 2018.

Ibrahim, M. A. A.; Moussa, N. A. M.; Safy, M. E. A.  
Quantum-mechanical investigation of tetrel bond characteristics based on the point-of-charge  
(PoC) approach  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3752-2

Iliev, S.; Gocheva, G.; Ivanova, N.; Atanasova, B.; Petrova, J.; Madjarova, G.; Ivanova, A.  
Identification and computational characterization of isomers with cis and trans amide bonds in  
folate and its analogues  
Physical Chemistry Chemical Physics, (20): 28818-28831. 2018. 10.1039/c8cp04304c

Illia, O.; Porcar-Tost, O.; Robledillo, C.; Elvira, C.; Nolis, P.; Reiser, O.; Branchadell, V.; Ortuno, R. M.  
Stereoselectivity of Proline/Cyclobutane Amino Acid-Containing Peptide Organocatalysts for  
Asymmetric Aldol Additions: A Rationale  
Journal of Organic Chemistry, (83): 350-363. 2018. 10.1021/acs.joc.7b02745

Inamdar, S. R.; Mannekutla, J. R.; Sannaikar, M. S.; Wari, M. N.; Mulimani, B. G.; Savadatti, M. I.  
Photophysics and rotational diffusion dynamics of large prolate non-polar laser dyes  
Journal of Molecular Liquids, (268): 66-76. 2018. 10.1016/j.molliq.2018.07.005

Ingrosso, F.; Ruiz-Lopez, M. F.  
Electronic Interactions in Iminophosphorane Superbase Complexes with Carbon Dioxide  
Journal of Physical Chemistry A, (122): 1764-1770. 2018. 10.1021/acs.jpca.7b11353

Iramain, M. A.; Davies, L.; Brandan, S. A.

Evaluating structures, properties and vibrational and electronic spectra of the potassium 2-isonicotinoyltrifluoroborate salt

Journal of Molecular Structure, (1163): 41-53. 2018. 10.1016/j.molstruc.2018.02.098

Iramain, M. A.; Davies, L.; Brandan, S. A.

FT-IR, FT-Raman and UV-visible spectra of potassium 3-furoyltrifluoroborate salt

Journal of Molecular Structure, (1158): 245-254. 2018. 10.1016/j.molstruc.2018.01.040

Iravani, M.; Omidyan, R.

Photochromism of 2-(2-Hydroxyphenyl) Benzothiazole (HBT) and Its Derivatives: A Theoretical Study

Journal of Physical Chemistry A, (122): 3182-3189. 2018. 10.1021/acs.jpca.8b00266

Isaev, A. N.

Ammonia and phosphine complexes with proton donors. Hydrogen bonding from the backside of the N(P) lone pair

Computational and Theoretical Chemistry, (1142): 28-38. 2018. 10.1016/j.comptc.2018.08.021

Isaev, A. N.

syn- and anti-H Bonds in Ammonia and Phosphine Complexes with Proton Donors

Russian Journal of Physical Chemistry A, (92): 1959-1969. 2018. 10.1134/s0036024418100096

Ishikawa, M.; Hirai, S.; Yoshida, T.; Shibuya, N.; Hama, S.; Takahashi, Y.; Fukuta, T.; Tanaka, T.; Hosoi, S.; Kogure, K.

Carotenoid Stereochemistry Affects Antioxidative Activity of Liposomes Co-encapsulating Astaxanthin and Tocotrienol

Chemical & Pharmaceutical Bulletin, (66): 714-720. 2018. 10.1248/cpb.c18-00035

Islam, M. S.; Barakat, A.; Al-Majid, A. M.; Soliman, S. M.; Ghabbour, H. A.; Shaik, M. R.; Ali, M.

Chemical reactivity, molecular structure, spectroscopic and DFT computational studies of spiro-heterocycle incorporating furan ring

Materials Express, (8): 335-344. 2018. 10.1166/mex.2018.1442

Ivanov, M. V.; Reid, S. A.; Rathore, R.

Game of Frontier Orbitals: A View on the Rational Design of Novel Charge-Transfer Materials

Journal of Physical Chemistry Letters, (9): 3978-3986. 2018. 10.1021/acs.jpcllett.8b01093

Ivanov, M. V.; Wang, D. N.; Rathore, R.

From Static to Dynamic: Electron Density of HOMO at Biaryl Linkage Controls the Mechanism of Hole Delocalization

Journal of the American Chemical Society, (140): 4765-4769. 2018. 10.1021/jacs.8b00466

- Ivanova, B.; Spiteller, M.  
Cation-pi-complex of Ag(I) ion with 1H-indole-5-carboxylic acid - Structural analysis and energetics of the M-L bonds  
*Inorganica Chimica Acta*, (471): 219-222. 2018. 10.1016/j.ica.2017.10.022
- Ivanova, L. V.; Navale, T. S.; Wang, D. N.; Lindeman, S.; Ivanov, M. V.; Rathore, R.  
Towards the rational design of novel charge-transfer materials: biaryls with a dihedral angle-independent hole delocalization mechanism  
*Chemical Communications*, (54): 5851-5854. 2018. 10.1039/c8cc02595a
- Ivanova, L. V.; Wang, D. A.; Lindeman, S.; Ivanov, M. V.; Rathore, R.  
Probing Charge Delocalization in Solid State Polychromophoric Cation Radicals Using X-ray Crystallography and DFT Calculations  
*Journal of Physical Chemistry C*, (122): 9339-9345. 2018. 10.1021/acs.jpcc.8b02184
- Ivlev, S. I.; Karttunen, A. J.; Buchner, M. R.; Conrad, M.; Kraus, F.  
The Interhalogen Cations Br<sub>2</sub>F<sub>5</sub> (+) and Br<sub>3</sub>F<sub>8</sub> (+)  
*Angewandte Chemie-International Edition*, (57): 14640-14644. 2018. 10.1002/anie.201803708
- Iwasaki, T.; Fukuoka, A.; Yokoyama, W.; Min, X.; Hisaki, I.; Yang, T.; Ehara, M.; Kuniyasu, H.; Kambe, N.  
Nickel-catalyzed coupling reaction of alkyl halides with aryl Grignard reagents in the presence of 1,3-butadiene: mechanistic studies of four-component coupling and competing cross-coupling reactions  
*Chemical Science*, (9): 2195-2211. 2018. 10.1039/57sc04675h
- Iwasaki, T.; Min, X.; Fukuoka, A.; Zhu, L. Z.; Qiu, R. H.; Yang, T.; Ehara, M.; Sudalai, A.; Kambe, N.  
Ni-Catalyzed Dimerization and Hydroperfluoroarylation of 1,3-Dienes  
*Journal of Organic Chemistry*, (83): 9267-9277. 2018. 10.1021/acs.joc.8b01266
- Iyanov, M. V.; Shukla, R.; Lindeman, S. V.; Wang, D. N.; Rathore, R.  
Pyrene-Like HOMO Governs Polaron Delocalization in Model Graphitic Strips: A Combined Experimental and Computational Analysis  
*Journal of Physical Chemistry C*, (122): 24527-24534. 2018. 10.1021/acs.jpcc.8b06068
- Iyer, A. H.; Deepak, R.; Sankararamakrishnan, R.  
Imidazole Nitrogens of Two Histidine Residues Participating in N-H center dot center dot center dot N Hydrogen Bonds in Protein Structures: Structural Bioinformatics Approach Combined with Quantum Chemical Calculations  
*Journal of Physical Chemistry B*, (122): 1205-1212. 2018. 10.1021/acs.jpcb.7b11737
- Izuogu, D. C.; Yoshida, T.; Zhang, H. T.; Cosquer, G.; Katoh, K.; Ogata, S.; Hasegawa, M.; Nojiri, H.; Damjanovic, M.; Wernsdorfer, W.; Uruga, T.; Ina, T.; Breedlove, B. K.; Yamashita, M.  
Slow Magnetic Relaxation in a Palladium-Gadolinium Complex Induced by Electron Density Donation from the Palladium Ion  
*Chemistry-a European Journal*, (24): 9285-9294. 2018. 10.1002/chem.201800699

Jablonski, M.

Hydride-Triel Bonds

Journal of Computational Chemistry, (39): 1177-1191. 2018. 10.1002/jcc.25178

Jafari, S.; Kazemi, N.; Ryde, U.; Irani, M.

Higher Flexibility of Glu-172 Explains the Unusual Stereospecificity of Glyoxalase I

Inorganic Chemistry, (57): 4944-4958. 2018. 10.1021/acs.inorgchem.7b03215

Jafari-Chermahini, M. T.; Tavakol, H.

Adsorption of CO<sub>2</sub> on sodium iodide (NaI)(n) (n <= 10) clusters: A density functional theory investigation

Computational and Theoretical Chemistry, (1145): 37-43. 2018. 10.1016/j.comptc.2018.10.009

Jafari-Moghaddam, F.; Beyramabadi, S. A.; Khashi, M.; Morsali, A.

Three VO<sub>2</sub><sup>+</sup> complexes of the pyridoxal-derived Schiff bases: Synthesis, experimental and theoretical characterizations, and catalytic activity in a cyclocondensation reaction

Journal of Molecular Structure, (1153): 149-156. 2018. 10.1016/j.molstruc.2017.10.007

Jagadeesan, R.; Sabapathi, G.; Madhavan, J.; Venuvanalingam, P.

Structure and Reactivity of Pd Complexes in Various Oxidation States in Identical Ligand Environments with Reference to C-C and C-Cl Coupling Reactions: Insights from Density Functional Theory

Inorganic Chemistry, (57): 6833-6846. 2018. 10.1021/acs.inorgchem.8b00239

Jagvaral, Y.; He, H. Y.; Pandey, R.

Interaction of silicene with amino acid analogues-from physical to chemical adsorption in gas and solvated phases

2d Materials, (5) 2018. 10.1088/2053-1583/aa8c92

Jain, R.; Al Mamun, A.; Buchanan, R. M.; Kozlowski, P. M.; Grapperhaus, C. A.

Ligand-Assisted Metal-Centered Electrocatalytic Hydrogen Evolution upon Reduction of a Bis(thiosemicarbazone)Ni(II) Complex

Inorganic Chemistry, (57): 13486-13493. 2018. 10.1021/acs.inorgchem.8b02110

Jana, G.; Pal, R.; Chattaraj, P. K.

Hydrogen storage in lithium adsorbed and polylithiated (OLi<sub>2</sub>) heteroatom (B, N) modified (2,2) gamma-graphyne nanotube and its CO sensing potential: A computational study

Journal of the Indian Chemical Society, (95): 1457-1464. 2018.

Jana, G.; Pan, S.; Merino, G.; Chattaraj, P. K.

Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au)

Journal of Physical Chemistry A, (122): 7391-7401. 2018. 10.1021/acs.jpca.8b05404

Jana, G.; Pan, S.; Osorio, E.; Zhao, L. L.; Merino, G.; Chattaraj, P. K.  
Cyanide-isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides  
(metal = Cu, Ag, Au)  
Physical Chemistry Chemical Physics, (20): 18491-18502. 2018. 10.1039/c8cp02837k

Jana, G.; Pan, S.; Rodriguez-Kessler, P. L.; Merino, G.; Chattaraj, P. K.  
Adsorption of Molecular Hydrogen on Lithium-Phosphorus Double-Helices  
Journal of Physical Chemistry C, (122): 27941-27946. 2018. 10.1021/acs.jpcc.8b09811

Jana, G. A.; Mendoza, F.; Osorio, M. I.; Alderete, J. B.; Fernandes, P. A.; Ramos, M. J.; Jimenez, V. A.  
A QM/MM approach on the structural and stereoelectronic factors governing glycosylation by  
GTF-SI from Streptococcus mutans  
Organic & Biomolecular Chemistry, (16): 2438-2447. 2018. 10.1039/c8ob00284c

Janesko, B. G.; Villegas, H.  
Attractive Nonbonded Interactions Help Stabilize the Z Form of Alkenyl Anions  
Journal of Organic Chemistry, (83): 8208-8213. 2018. 10.1021/acs.joc.8b00960

Jankowski, P.; Poterala, M.; Lindahl, N.; Wieczorek, W.; Johansson, P.  
Chemically soft solid electrolyte interphase forming additives for lithium-ion batteries  
Journal of Materials Chemistry A, (6): 22609-22618. 2018. 10.1039/c8ta07936f

Jasiewicz, B.; Sierakowska, A.; Jankowski, W.; Hoffmann, M.; Pioronska, W.; Gornicka, A.; Bielawska, A.;  
Bielawski, K.; Mrowczynska, L.  
Antioxidant and cytotoxic activity of new di- and polyamine caffeine analogues  
Free Radical Research, (52): 724-736. 2018. 10.1080/10715762.2018.1467561

Jassal, A. K.; Sran, B. S.; Mandal, K.; Mukhopadhyay, P.; Hundal, G.  
Role Reversal of the Carboxylate Group from Coordination to Hydrogen Bonding Only, in  
Structurally Diverse Metal-2-amino,5-Nitro-benzoates: A First Report  
Crystal Growth & Design, (18): 4737-4748. 2018. 10.1021/acs.cgd.8b00771

Javadi, N.; Vatanparast, M.  
Potential application of doped hexa-peri-hexabenzocoronene as NH<sub>3</sub> gas sensor: a  
computational investigation  
Structural Chemistry, (29): 929-935. 2018. 10.1007/s11224-018-1076-6

Jayakody, R. S.; Wijewardhane, P.; Herath, C.; Perera, S.  
Bergenin: a computationally proven promising scaffold for novel galectin-3 inhibitors  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3831-4

Jayakumar, K.; Camarada, M. B.; Dharuman, V.; Rajesh, R.; Venkatesan, R.; Ju, H. X.; Maniraj, M.; Rai, A.;  
Barman, S. R.; Wen, Y. P.

Layer-by-Layer-Assembled AuNPs-Decorated First-Generation Poly(amidoamine) Dendrimer with Reduced Graphene Oxide Core as Highly Sensitive Biosensing Platform with Controllable 3D Nanoarchitecture for Rapid Voltammetric Analysis of Ultratrace DNA Hybridization  
ACS Applied Materials & Interfaces, (10): 21541-21555. 2018. 10.1021/acsami.8b03236

Jayasheela, K.; Al-Wahaibi, L. H.; Periandy, S.; Hassan, H. M.; Sebastian, S.; Xavier, S.; Daniel, J. C.; El-Emam, A. A.; Attia, M. I.

Probing vibrational activities, electronic properties, molecular docking and Hirshfeld surfaces analysis of 4-chlorophenyl ({(1E)-3-(1H-imidazol-1-yl)-1-phenylpropylidene amino}oxy)methanone: A promising anti-Candida agent

Journal of Molecular Structure, (1159): 83-95. 2018. 10.1016/j.molstruc.2018.01.042

Jayasree, E. G.; Sreedevi, S.

Computational study on ionic and ion pair methylation reactions of enethiolates and their lithium salts

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2379-9

Jensen, K. T.; Benson, R. L.; Cardamone, S.; Thom, A. J. W.

Modeling Electron Transfers Using Quasidiabatic Hartree-Fock States

Journal of Chemical Theory and Computation, (14): 4629-4639. 2018. 10.1021/acs.jctc.8b00379

Jerabek, P.; Vondung, L.; Schwerdtfeger, P.

Tipping the Balance between Ligand and Metal Protonation due to Relativistic Effects: Unusually High Proton Affinity in Gold(I) Pincer Complexes

Chemistry-a European Journal, (24): 6047-6051. 2018. 10.1002/chem.201800755

Jeremic, S.; Tran, T. H.; Markovic, Z.; Ngo, T. C.; Dao, D. Q.

Insight into interaction properties between mercury and lead cations with chitosan and chitin: Density functional theory studies

Computational and Theoretical Chemistry, (1138): 99-106. 2018. 10.1016/j.comptc.2018.06.010

Jerez, A. L. P.; Robles, N. L.

On the search of cumulative effect of fluoro-substituents in the structural and vibrational properties of sulfinylanilines: Study of 3,4-difluorosulfinylaniline and 2,3,4-trifluorosulfinylaniline

Journal of Fluorine Chemistry, (213): 1-10. 2018. 10.1016/j.jfluchem.2018.06.007

Jeyavijayan, S.; Gobinath, E.; Viswanathan, K.; Kumar, J. S.

Vibrational spectroscopic investigations, DFT computations, nonlinear optical and other molecular properties of 3-bromo-5-fluorobenzonitrile

Indian Journal of Pure & Applied Physics, (56): 108-118. 2018.

Jia, Q. Q.; Li, Q. Z.; Luo, M.; Li, H. B.

Understanding the effects of vicinal carbon substituents and configuration on organofluorine hydrogen-bonding interaction

RSC Advances, (8): 38980-38986. 2018. 10.1039/c8ra08122k

Jia, X. L.; Li, C. Z.; Li, D. L.; Liu, Y. F.

TDDFT study on excited state intramolecular proton transfer mechanism in 2-amino-3-(2'-benzazoly1)-quinolines

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (192): 168-173. 2018. 10.1016/j.saa.2017.11.021

Jiang, B.; Zhao, M.; Li, S. S.; Xu, Y. H.; Loh, T. P.

Macrolide Synthesis through Intramolecular Oxidative Cross-Coupling of Alkenes

Angewandte Chemie-International Edition, (57): 555-559. 2018. 10.1002/anie.201710601

Jiang, H. Y.; Li, Q.; Qi, Q. J.; Yang, C. X.; Zhang, D.

Theoretical Study on the Conjugate Addition of Asymmetric Michael Addition of trans-1-Nitro-2-phenylethylene to 2-Methylpropion-aldehyde Catalyzed by Cinchona Alkaloid Derived Primary Amine

Chinese Journal of Organic Chemistry, (38): 825-831. 2018. 10.6023/cjoc201703037

Jiang, L. H.; Huang, F.; Wang, Q.; Sun, C. Z.; Liu, J. B.; Chen, D. Z.

Mechanistic insight into Ni-mediated decarbonylation of unstrained ketones: the origin of decarbonylation catalytic activity

Organic Chemistry Frontiers, (5): 2332-2339. 2018. 10.1039/c8qo00335a

Jiang, X. K.; Zhang, J. J.; Zhou, B.; Li, P.; Hu, X. J.; Zhu, Z.; Tan, Y. W.; Chang, C.; Lu, J. H.; Song, B.

Anomalous behavior of membrane fluidity caused by copper-copper bond coupled phospholipids

Scientific Reports, (8) 2018. 10.1038/s41598-018-32322-4

Jiang, X. Y.; Wu, W.; Mo, Y. R.

Strength of Intramolecular Hydrogen Bonds

Acta Physico-Chimica Sinica, (34): 278-285. 2018. 10.3866/pku.Whxb201708174

Jiang, Y.; Xue, Y.; Zeng, Y.

Microsolvated Model for the Kinetics and Thermodynamics of Glycosidic Bond Dissociative Cleavage of Nucleoside D4G

Journal of Physical Chemistry B, (122): 1816-1825. 2018. 10.1021/acs.jpcb.7b11331

Jiang, Y. H.; Wang, D. S.; Xu, D.; Zhang, J. Y.; Wang, Z. Y.

Dimerization of Metallofullerenes to Obtain Materials with Enhanced Nonlinear Optical Properties

Chemphyschem, (19): 2995-3000. 2018. 10.1002/cphc.201800797

Jiang, Y. Y.; Liu, T. T.; Sun, X.; Xu, Z. Y.; Fan, X.; Zhu, L.; Bi, S. W.

Computational study of the mechanism of amide bond formation via CS<sub>2</sub>-releasing 1,3-acyl transfer

Organic & Biomolecular Chemistry, (16): 5808-5815. 2018. 10.1039/c8ob01338a

Jiang, Y. Y.; Liu, T. T.; Zhang, R. X.; Xu, Z. Y.; Sun, X.; Bi, S. W.

Mechanism and Rate-Determining Factors of Amide Bond Formation through Acyl Transfer of Mixed Carboxylic-Carbamic Anhydrides: A Computational Study

Journal of Organic Chemistry, (83): 2676-2685. 2018. 10.1021/acs.joc.7b03107

Jiao, C. X.; Qin, Z. B.; Cong, R.; Zheng, X. F.; Cui, Z. F.; Xie, H.; Tang, Z. C.

A comparative study on the bond features in CO, CS, and PbS

Journal of Chemical Physics, (149) 2018. 10.1063/1.5067006

Jilal, I.; El Barkany, S.; Bahari, Z.; Sundman, O.; El Idrissi, A.; Salhi, A.; Abou-Salama, M.; Loutou, M.; Amhamdi, H.

Unconventional synthesis, characterization and theoretical study (HF and DFT computations) of new cellulosic copper complex: benzyloxyethyl cellulose copper (CuBEC)

Cellulose, (25): 4375-4388. 2018. 10.1007/s10570-018-1909-x

Jin, L. X.; Shi, S. N.; Zhao, Y.; Luo, L. Y.; Zhao, C. B.; Lu, J. F.; Jiang, M.

Effects of C5-substituent group on the hydrogen peroxide-mediated tautomerisation of protonated cytosine: a theoretical perspective

Molecular Physics, (116): 471-481. 2018. 10.1080/00268976.2017.1406159

Jin, Q.; Jin, B.; Zhang, Z. H.; He, X. N.

AROMATICITY OF BARE IRIDIUM TRIMERS AND Ir<sub>3</sub>M0/+ AND Ir<sub>3</sub>M2+ (M = Li, Na, K, and Be, Ca)

BIMETALLIC CLUSTERS

Journal of Structural Chemistry, (59): 1032-1043. 2018. 10.1134/s0022476618050049

Jin, S.; Hu, Y. J.; Wang, P. C.; Zhan, H. Q.; Lu, O.; Liu, F. Y.; Sheng, L. S.

Hydrogen bonding and dominant conformations of hydrated sugar analogue complexes using tetrahydrofurfuryl alcohol as the model sugar molecule

Physical Chemistry Chemical Physics, (20): 7351-7360. 2018. 10.1039/c7cp07935d

John, J. S.; Sajan, D.; Narayana, C.; Joy, N.; Philip, R.

Theoretical and experimental approach to the investigation of hyperpolarizability and charge transfer characteristics of NLO active 2',3,4, 4',5-pentamethoxy chalcone with silver atoms adsorbed

Optical Materials, (84): 409-421. 2018. 10.1016/j.optmat.2018.07.1336

John, J. S.; Sajan, D.; Narayana, C.; Sundius, T.

Optical nonlinearity and charge transfer analysis of 4- (E)-2-(2,4,6-Trinitrophenyl) ethylidene benzonitrile adsorbed on silver nanoparticles: Computational and experimental investigations

Optics and Laser Technology, (107): 454-467. 2018. 10.1016/j.optlastec.2018.06.006

John, N. L.; Joy, L. K.; Kumar, M. S.; Shaiju, S. S.; Subashini, A.; Sajan, D.

Quantitative structure and activity relationship on the biological, nonlinear and the spectroscopic properties of the Schiff base material: 4-chloro-4bromobenzylidene aniline  
Molecular Simulation, (44): 40-54. 2018. 10.1080/08927022.2017.1337272

Johnson, M. A.; Flinn, C.; Zhao, Y. M.

Computational Mechanistic Analysis of Intramolecular Cycloadditions of the 1,3-Dithiolium Cation with Adjacent Alkene and Allene Functional Groups  
ACS Omega, (3): 9770-9780. 2018. 10.1021/acsomega.8b01332

Johnstone, T. C.; Briceno-Strocchia, A. I.; Stephan, D. W.

Frustrated Lewis Pair Oxidation Permits Synthesis of a Fluoroazaphosphatrane,  
FP(MeNCH<sub>2</sub>CH<sub>2</sub>)(3)N (+)  
Inorganic Chemistry, (57): 15299-15304. 2018. 10.1021/acs.inorgchem.8b02605

Jolleys, A.; Lake, B. R. M.; Kramer, T.; Benjamin, S. L.

A Five-Membered PdSb<sub>n</sub> Coordination Series  
Organometallics, (37): 3854-3862. 2018. 10.1021/acs.organomet.8b00556

Jorner, K.; Jahn, B. O.; Bultinck, P.; Ottosson, H.

Triplet state homoaromaticity: concept, computational validation and experimental relevance  
Chemical Science, (9): 3165-3176. 2018. 10.1039/c7sc05009g

Joseph, B.; Barik, S. K.; Ramalakshmi, R.; Kundu, G.; Roisnel, T.; Dorcet, V.; Ghosh, S.

Chemistry of Triple-Decker Sandwich Complexes Containing Four-Membered Open B<sub>2</sub>E<sub>2</sub> Rings  
(E = S or Se)

European Journal of Inorganic Chemistry: 2045-2053. 2018. 10.1002/ejic.201800371

Joseph, B.; Gomosta, S.; Barik, S. K.; Sinha, S. K.; Roisnel, T.; Dorcet, V.; Halet, J. F.; Ghosh, S.

Synthesis and characterization of diruthenaborane analogues of pentaborane(11) and hexaborane(10)

Journal of Organometallic Chemistry, (865): 29-36. 2018. 10.1016/j.jorgchem.2017.12.011

Joseph, B.; Saha, K.; Prakash, R.; Nandi, C.; Roisnel, T.; Ghosh, S.

Chalcogenolato-bridged dinuclear half sandwich complexes of ruthenium and iridium  
Inorganica Chimica Acta, (483): 106-110. 2018. 10.1016/j.ica.2018.08.005

Joshi, B. D.; Srivastava, A.; Tandon, P.; Jain, S.; Ayala, A. P.

A combined experimental (IR, Raman and UV-Vis) and quantum chemical study of canadine  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (191): 249-258. 2018.  
10.1016/j.saa.2017.10.008

Joshi, M.; Chandrasekar, A.; Ghanty, T. K.

Theoretical investigation of M@Pb-12(2-) and M@Sn-12(2-) Zintl clusters (M = Lrn+, Lun+, La3+, Ac3+ and n=0, 1, 2, 3)

Physical Chemistry Chemical Physics, (20): 15253-15272. 2018. 10.1039/c8cp01056k

Joshi, M.; Ghanty, T. K.

Hybrid Organic-Inorganic Functionalized Dodecaboranes and Their Potential Role in Lithium and Magnesium Ion Batteries

Journal of Physical Chemistry C, (122): 27947-27954. 2018. 10.1021/acs.jpcc.8b09850

Joshi, M.; Ghosh, A.; Chandrasekar, A.; Ghanty, T. K.

Counter-Intuitive Stability in Actinide-Encapsulated Metalloid Clusters with Broken Aromaticity

Journal of Physical Chemistry C, (122): 22469-22479. 2018. 10.1021/acs.jpcc.8b05883

Joshi, R.; Pandey, N.; Yadav, S. K.; Tilak, R.; Mishra, H.; Pokharia, S.

Synthesis, spectroscopic characterization, DFT studies and antifungal activity of (E)-4-amino-5-N'-(2-nitro-benzylidene)-hydrazino -2,4-dihydro- 1,2,4 triazole-3-thione

Journal of Molecular Structure, (1164): 386-403. 2018. 10.1016/j.molstruc.2018.03.081

Joshi, R.; Yadav, S. K.; Mishra, H.; Pandey, N.; Tilak, R.; Pokharia, S.

Interaction of triorganotin(IV) moiety with quinolone antibacterial drug ciprofloxacin: Synthesis, spectroscopic investigation, electronic structure calculation, and biological evaluation

Heteroatom Chemistry, (29) 2018. 10.1002/hc.21433

Jouypazadeh, H.; Farrokhpour, H.

DFT and TD-DFT study of the adsorption and detection of sulfur mustard chemical warfare agent by the C-24, C12Si12, Al12N12, Al12P12, Be12O12, B12N12 and Mg12O12 nanocages

Journal of Molecular Structure, (1164): 227-238. 2018. 10.1016/j.molstruc.2018.03.051

Joy, J.; Akhil, E.; Jemmis, E. D.

Halogen bond shortens and strengthens the bridge bond of 1.1.1 propellane and the open form of 2.2.2 propellane

Physical Chemistry Chemical Physics, (20): 25792-25798. 2018. 10.1039/c8cp05125a

Joy, L. K.; George, M.; Alex, J.; Aravind, A.; Sajan, D.; Vinitha, G.

Twisted intramolecular charge transfer investigation of semi organic L-Glutamic acid hydrochloride single crystal for organic light-emitting and optical limiting applications

Journal of Molecular Structure, (1156): 733-744. 2018. 10.1016/j.molstruc.2017.11.126

Joy, M.; Anabha, E. R.; Gopi, S.; Mathew, B.; Kumar, S. A.; Mathews, A.

Structural and optical profile of a multifunctionalized 2-pyridone derivative in a crystal engineering perspective

Acta Crystallographica Section C-Structural Chemistry, (74): 807-+. 2018.

10.1107/s2053229618007490

Joy, S.; Sureshbabu, V. V.; Periyasamy, G.

Computational studies on ground and excited state charge transfer properties of peptidomimetics

Faraday Discussions, (207): 77-90. 2018. 10.1039/c7fd00183e

Ju, Z. Y.; Xiao, W. H.; Lu, X. M.; Liu, X. M.; Yao, X. Q.; Zhang, X. C.; Zhang, S. J.

Theoretical studies on glycolysis of poly(ethylene terephthalate) in ionic liquids

RSC Advances, (8): 8209-8219. 2018. 10.1039/c7ra13173a

Juaristi, E.; Notario, R.

Density Functional Theory Computational Reexamination of the Anomeric Effect in 2-Methoxy- and 2-Cyano-1,3-dioxanes and 1,3-Dithianes. Stereoelectronic Interactions Involving the Cyano (C N:) Group Revealed by Natural Bond Orbital (NBO) Analysis

Journal of Organic Chemistry, (83): 10326-10333. 2018. 10.1021/acs.joc.8b01458

Juaristi, E.; Notario, R.

Stereoelectronic Interactions Exhibited by (1)J(C-H) One-Bond Coupling Constants and Examination of the Possible Existence of the Intramolecular alpha-Effect in Six-Membered Oxygen-Containing Heterocycles

Journal of Organic Chemistry, (83): 3293-3298. 2018. 10.1021/acs.joc.8b00220

Jung, H.; Kang, J.; Chun, H.; Han, B.

First principles computational study on hydrolysis of hazardous chemicals phosphorus trichloride and oxychloride (PC3 and POCl3) catalyzed by molecular water clusters

Journal of Hazardous Materials, (341): 457-463. 2018. 10.1016/j.jhazmat.2017.08.054

Jung, R.; Strobl, P.; Maglia, F.; Stinner, C.; Gasteiger, H. A.

Temperature Dependence of Oxygen Release from LiNi0.6Mn0.2Co0.2O2 (NMC622) Cathode Materials for Li-Ion Batteries

Journal of the Electrochemical Society, (165): A2869-A2879. 2018. 10.1149/2.1261811jes

Jung, S.; Podlech, J.

Stereoelectronic Effects: The gamma-Gauche Effect in Sulfoxides

Journal of Physical Chemistry A, (122): 5764-5772. 2018. 10.1021/acs.jpca.8b03729

Jungen, S.; Chen, P.

Alkyl Radical Generation by an Intramolecular Homolytic Substitution Reaction between Iron(II) and Trialkylsulfonium Groups

Chemistry-a European Journal, (24): 11008-11020. 2018. 10.1002/chem.201801952

Kabanda, M. M.; Serobatse, K. R. N.

A DFT study on the addition and abstraction reactions of thiourea with hydroxyl radical

Journal of Sulfur Chemistry, (39): 23-46. 2018. 10.1080/17415993.2017.1359269

Kachwal, V.; Krishna, I. S. V.; Fageria, L.; Chaudhary, J.; Roy, R. K.; Chowdhury, R.; Laskar, I. R.

Exploring the hidden potential of a benzothiazole-based Schiff-base exhibiting AIE and ESIPT and its activity in pH sensing, intracellular imaging and ultrasensitive & selective detection of aluminium (Al<sup>3+</sup>)

Analyst, (143): 3741-3748. 2018. 10.1039/c8an00349a

Kadela-Tomanek, M.; Pawelczak, B.; Jastrzbska, M.; Bgbenek, E.; Chrobak, E.; Latocha, M.; Kusz, J.; Ksieki, M.; Boryczka, S.

Structural, vibrational and quantum chemical investigations for 6,7dichloro-2-methyl-5,8-quinolinedione. Cytotoxic and molecular docking studies

Journal of Molecular Structure, (1168): 73-83. 2018. 10.1016/j.molstruc.2018.05.031

Kalinowska, M.; Bajko, E.; Matejczyk, M.; Kaczynski, P.; Lozowicka, B.; Lewandowski, W.

The Study of Anti-/Pro-Oxidant, Lipophilic, Microbial and Spectroscopic Properties of New Alkali Metal Salts of 5-O-Caffeoylquinic Acid

International Journal of Molecular Sciences, (19) 2018. 10.3390/ijms19020463

Kamel, M.; Raissi, H.; Morsali, A.; Shahabi, M.

Assessment of the adsorption mechanism of Flutamide anticancer drug on the functionalized single-walled carbon nanotube surface as a drug delivery vehicle: An alternative theoretical approach based on DFT and MD

Applied Surface Science, (434): 492-503. 2018. 10.1016/j.apsusc.2017.10.165

Kanagathara, N.; Pawlus, K.; Marchewka, M. K.

Vibrational Spectroscopic and Computational Studies on Bis(2-aminopyridinium)fumarate - Fumaric Acid (1:1) Complex

Acta Physica Polonica A, (133): 45-56. 2018. 10.12693/APhysPolA.133.45

Kaneko, M.; Suzuki, H.; Matsumura, T.

Theoretical Elucidation of Am(III)/Cm(III) Separation Mechanism with Diamide-type Ligands Using Relativistic Density Functional Theory Calculation

Inorganic Chemistry, (57): 14513-14523. 2018. 10.1021/acs.inorgchem.8b01624

Kaplan, I. G.; Miranda, U.; Trakhtenberg, L. I.

Study of the In<sub>2</sub>O<sub>3</sub> molecule in the free state and in the crystal

Molecular Physics, (116): 678-685. 2018. 10.1080/00268976.2017.1414963

Kar, S.; Saha, K.; Saha, S.; Kirubakaran, B.; Dorcet, V.; Ghosh, S.

Trimetallic Cubane-Type Clusters: Transition-Metal Variation as a Probe of the Roots of Hypoelectronic Metallaheteroboranes

Inorganic Chemistry, (57): 10896-10905. 2018. 10.1021/acs.inorgchem.8b01531

Karabiyik, H.; Urut, G. O.; Sevincer, R.

Excited state aromatization assisted push-pull abilities of two unsaturated oxazolone derivatives

Journal of Saudi Chemical Society, (22): 519-526. 2018. 10.1016/j.jscs.2017.09.001

- Karakus, M.; Kara, I.; Celik, O.; Orujalipoor, I.; Ide, S.; Yilmaz, H.  
Synthesis, characterization, single crystal structure and theoretical studies of trans-Ni(II)-complex with dithiophosphonate ligand  
Journal of Molecular Structure, (1163): 128-136. 2018. 10.1016/j.molstruc.2018.02.110
- Karasmani, F.; Tsipis, A.; Angaridis, P.; Hatzidimitriou, A. G.; Aslanidis, P.  
Experimental and spin-orbit coupled TDDFT predictions of photophysical properties of three-coordinate mononuclear and four-coordinate binuclear copper(I) complexes with thioamidines and bulky triarylphosphanes  
Inorganica Chimica Acta, (471): 680-690. 2018. 10.1016/j.ica.2017.12.002
- Karimzadeh, M.; Asl, H. S.; Hashemi, H.; Saberi, D.; Niknam, K.  
Base-free benzylation of 1,3-dicarbonyl compounds using sulfamic acid supported on silica by linker: a combined experimental and theoretical approach  
Monatshefte fur Chemie, (149): 2237-2244. 2018. 10.1007/s00706-018-2284-x
- Karir, G.; Kumar, G.; Kar, B. P.; Viswanathan, K. S.  
Multiple Hydrogen Bond Tethers for Grazing Formic Acid in Its Complexes with Phenylacetylene  
Journal of Physical Chemistry A, (122): 2046-2059. 2018. 10.1021/acs.jpca.7b11428
- Kashefolgheta, S.; Verde, A. V.  
Developing force fields when experimental data is sparse: AMBER/GAFF-compatible parameters for inorganic and alkyl oxoanions (vol 19, pg 20593, 2017)  
Physical Chemistry Chemical Physics, (20): 28346-28347. 2018. 10.1039/c8cp91863e
- Kaur, D.; Kaur, R.; Chopra, G.  
Comparison of hydrogen- and halogen-bonding interactions in the complexes of the substituted carbonyl compounds with hypohalous acids and monohaloamines  
Structural Chemistry, (29): 207-215. 2018. 10.1007/s11224-017-1020-1
- Kaur, R.; Rani, N.; Vikas  
Gas-Phase Stereoinversion in Aspartic Acid: Reaction Pathways, Computational Spectroscopic Analysis, and Its Astrophysical Relevance  
ACS Omega, (3): 14431-14447. 2018. 10.1021/acsomega.8b01721
- Kausteklis, J.; Aleksa, V.; Iramain, M. A.; Brandan, S. A.  
Effect of cation-anion interactions on the structural and vibrational properties of 1-butyl-3-methyl imidazolium nitrate ionic liquid  
Journal of Molecular Structure, (1164): 563-576. 2018. 10.1016/j.molstruc.2018.03.100
- Kaviani, S.; Izadyar, M.  
The possibility of iron chelation therapy in the presence of different HPOs; a molecular approach to the non-covalent interactions and binding energies

Journal of Molecular Structure, (1166): 448-455. 2018. 10.1016/j.molstruc.2018.04.065

Kaviani, S.; Izadyar, M.; Housaindokht, M. R.

DFT investigation on the selective complexation of Fe<sup>3+</sup> and Al<sup>3+</sup> with hydroxypyridinones used for treatment of the aluminium and iron overload diseases

Journal of Molecular Graphics & Modelling, (80): 182-189. 2018. 10.1016/j.jmgm.2018.01.003

Kavimani, M.; Balachandran, V.; Narayana, B.; Vanasundari, K.; Revathi, B.

Topological analysis (BCP) of vibrational spectroscopic studies, docking, RDG, DSSC, Fukui functions and chemical reactivity of 2-methylphenylacetic acid

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (190): 47-60. 2018. 10.1016/j.saa.2017.09.005

Kavitha, T.; Velraj, G.

Molecular structure, spectroscopic and docking analysis of 1,3-diphenylpyrazole-4-propionic acid: A good prostaglandin reductase inhibitor

Journal of Molecular Structure, (1155): 819-830. 2018. 10.1016/j.molstruc.2017.11.031

Kavousi, H.; Rezaeifard, A.; Raeisi, H.; Jafarpour, M.

Screening of different interactions in oxo-manganese porphyrin dimers containing axial N-donor ligands: a theoretical study

RSC Advances, (8): 9770-9774. 2018. 10.1039/c8ra00540k

Kawamata, T.; Yamaguchi, A.; Nagatomo, M.; Inoue, M.

Convergent Total Synthesis of Asimicin via Decarbonylative Radical Dimerization  
Chemistry-a European Journal, (24): 18907-18912. 2018. 10.1002/chem.201805317

Kawashima, Y.; Iwano, S.; Hirota, E.

Fourier Transform Microwave Spectra of the Nitrogen Molecule-Ethylene Sulfide and Nitrogen Molecule-Dimethyl Sulfide Complexes

Journal of Physical Chemistry A, (122): 9454-9463. 2018. 10.1021/acs.jpca.8b08647

Keypour, H.; Mahmoudabadi, M.; Shooshtari, A.; Bayat, M.; Karamian, R.; Asadbegy, M.; Gable, R. W.

Synthesis, crystal structure, theoretical studies and biological properties of three novel trigonal prismatic Co(II), Ni(II) and Cu(II) macroacyclic Schiff base complexes incorporating piperazine moiety

Inorganica Chimica Acta, (478): 176-186. 2018. 10.1016/j.ica.2018.02.028

Keypour, H.; Mahmoudabadi, M.; Shooshtari, A.; Bayat, M.; Mohsenzadeh, F.; Gable, R. W.

Cadmium (II) macrocyclic Schiff-base complexes containing piperazine moiety: Synthesis, spectroscopic, X-ray structure, theoretical and antibacterial studies

Journal of Molecular Structure, (1155): 196-204. 2018. 10.1016/j.molstruc.2017.10.074

Khajehali, Z.; Shamlouei, H. R.

Structural, electrical and optical properties of Li-n@C-20 (n=1-6) nanoclusters

Comptes Rendus Chimie, (21): 541-546. 2018. 10.1016/j.crci.2018.02.005

Khajehzadeh, M.; Sadeghi, N.

Molecular structure, the effect of solvent on UV-vis and NMR, FT-IR and FT-Raman spectra, NBO, frontier molecular orbital analysis of Mitomycin anticancer drug

Journal of Molecular Liquids, (256): 238-246. 2018. 10.1016/j.molliq.2018.01.099

Khalid, M.; Ullah, R. S.; Choudhary, M. A.; Tahir, M. N.; Murtaza, S.; MunawarHussain; BakhatAli; ZahoorAhmed

Structural, SC-XRD and spectroscopic investigation of schiff base derivatives: A joint experimental and DFT investigation

Journal of Molecular Structure, (1167): 57-68. 2018. 10.1016/j.molstruc.2018.04.084

Khalili, B.

Structural and energetic quantum chemical investigations into how the bioactive thiazolidinedione and rhodanine scaffolds interact with cytosine to form part of DNA

Computational and Theoretical Chemistry, (1125): 1-14. 2018. 10.1016/j.comptc.2017.12.012

Khalili, B.; Rimaz, M.

A quantum chemical study of the interactions of uracil as a constituent of ribonucleic acid (RNA) with thiazolidinedione and rhodanine bioactive molecules: an insight into energetic and structural features

Structural Chemistry, (29): 681-702. 2018. 10.1007/s11224-017-1062-4

Khamees, H. A.; Jyothi, M.; Khanum, S. A.; Madegowda, M.

Synthesis, crystal structure, spectroscopic characterization, docking simulation and density functional studies of 1-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl)-propan-1-one

Journal of Molecular Structure, (1161): 199-217. 2018. 10.1016/j.molstruc.2018.02.045

Khan, M. S.; Pal, S.

Quantum mechanical studies on dioxin-imprinted polymer precursor composites: Fundamental insights to enhance the binding strength and selectivity of biomarkers

Journal of Molecular Recognition, (31) 2018. 10.1002/jmr.2736

Khan, M. U.; Khalid, M.; Ibrahim, M.; Braga, A. A. C.; Safdar, M.; Al-Saadi, A. A.; Janjua, M.

First Theoretical Framework of Triphenylamine-Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of pi-Linkers

Journal of Physical Chemistry C, (122): 4009-4018. 2018. 10.1021/acs.jpcc.7b12293

Khan, S. A.; Asiri, A. M.; Al-Dies, A. A. M.; Osman, O. I.; Asad, M.; Zayed, M. E. M.

One-pot synthesis, physicochemical and photophysical properties of deep blue light-emitting highly fluorescent pyrene-imidazole dye: A combined experimental and theoretical study

Journal of Photochemistry and Photobiology a-Chemistry, (364): 390-399. 2018.  
10.1016/j.jphotochem.2018.06.015

- Khani, S.; Montazerzohori, M.; Masoudiasl, A.; White, J. M.  
A new 1D manganese(II) coordination polymer with end-to-end azide bridge and  
isonicotinoylhydrazone Schiff base ligand: Crystal structure, Hirshfeld surface, NBO and thermal analyses  
*Journal of Molecular Structure*, (1153): 239-247. 2018. 10.1016/j.molstruc.2017.10.021
- Khavani, M.; Izadyar, M.; Housaindokht, M. R.  
DFT study on the selective complexation of B12N12 nanocage with alkali metal ions  
*Phosphorus Sulfur and Silicon and the Related Elements*, (193): 178-184. 2018.  
10.1080/10426507.2017.1394301
- Khavani, M.; Izadyar, M.; Housaindokht, M. R.  
Modeling of the Functionalized Gold Nanoparticle Aggregation in the Presence of Dopamine: A  
Joint MD/QM Study  
*Journal of Physical Chemistry C*, (122): 26130-26141. 2018. 10.1021/acs.jpcc.8b06600
- Khavani, M.; Kalantarinezhad, R.; Izadyar, M.  
A joint QM/MD study on alpha-, beta- and gamma-cyclodextrins in selective complexation with  
cathinone  
*Supramolecular Chemistry*, (30): 687-696. 2018. 10.1080/10610278.2018.1444764
- Khazaei, S.; Eskandari, M.; Zakavi, S.  
Computational and experimental insights into the oxidative stability of iron porphyrins: A mono-  
ortho-substituted iron porphyrin with unusually high oxidative stability  
*Journal of Physical Organic Chemistry*, (31) 2018. 10.1002/poc.3869
- Kheirabadi, R.; Izadyar, M.  
Antioxidant activity of selenenamide-based mimic as a function of the aromatic thiols  
nucleophilicity, a DFT-SAPE model  
*Computational Biology and Chemistry*, (75): 213-221. 2018.  
10.1016/j.compbiolchem.2018.05.017
- Kheirabadi, R.; Izadyar, M.; Housaindokht, M. R.  
Computational Kinetic Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic:  
Effect of Nucleophilicity of Thiols on the Catalytic Activity  
*Journal of Physical Chemistry A*, (122): 364-374. 2018. 10.1021/acs.jpca.7b09929
- Kheirjou, S.; Fattahi, A.  
Ionic liquid based on 6-amino-6-deoxy hexopyranose cation and BF4-, PF6-, and ClO4- as anions:  
A DFT study on the structural and electronic properties  
*Journal of Physical Organic Chemistry*, (31) 2018. 10.1002/poc.3798
- Kilgore, H. R.; Raines, R. T.

$n \rightarrow \pi^*$  Interactions Modulate the Properties of Cysteine Residues and Disulfide Bonds in Proteins

Journal of the American Chemical Society, (140): 17606-17611. 2018. 10.1021/jacs.8b09701

Kim, D. Y.; Yang, D. C.; Madridejos, J. M. L.; Hajibabaei, A.; Baig, C.; Kim, K. S.

Anisotropic and amphoteric characteristics of diverse carbenes

Physical Chemistry Chemical Physics, (20): 13722-13733. 2018. 10.1039/c8cp00457a

Kim, J. Y.; Kuik, H. J.

When Is Ligand pK(a) a Good Descriptor for Catalyst Energetics? In Search of Optimal CO<sub>2</sub> Hydration Catalysts

Journal of Physical Chemistry A, (122): 4579-4590. 2018. 10.1021/acs.jpca.8b03301

Kimura, A.; Ishida, T.

Spin-Crossover Temperature Predictable from DFT Calculation for Iron(II) Complexes with 4-Substituted Pybox and Related Heteroaromatic Ligands

ACS Omega, (3): 6737-6747. 2018. 10.1021/acsomega.8b01095

Kimura, T.; Kaneko, M.; Watanabe, M.; Miyashita, S.; Nakashima, S.

Computational chemical analysis of Eu(iii) and Am(iii) complexes with pnictogen-donor ligands using DFT calculations

Dalton Transactions, (47) 2018. 10.1039/c8dt01973h

Kinzhalov, M. A.; Katkova, S. A.; Doronina, E. P.; Novikov, A. S.; Eliseev, II; Ilichev, V. A.; Kukinov, A. A.; Starova, G. L.; Bokach, N. A.

Red photo- and electroluminescent half-lantern cyclometalated dinuclear platinum(II) complex

Zeitschrift Fur Kristallographie-Crystalline Materials, (233): 795-802. 2018. 10.1515/zkri-2018-2075

Kirana, K.; Gangadhar, V.; Prasad, G.

Synthesis and Characterization of Sodium Potassium Niobate and Cobalt Ferrite Multiferroic Composites

Transactions of the Indian Ceramic Society, (77): 100-105. 2018.

10.1080/0371750x.2018.1465359

Kireev, N. V.; Filippov, O. A.; Pavlov, A. A.; Epstein, L. M.; Makhaey, V. D.; Dyadchenko, V. P.; Shubina, E. S.; Belkova, N. V.

Steric and Acidity Control in Hydrogen Bonding and Proton Transfer to trans-W(N-2)(2)(dppe)(2)

Inorganic Chemistry, (57): 1656-1664. 2018. 10.1021/acs.inorgchem.7b03027

Kirpichenko, S. V.; Shainyan, B. A.; Kleinpeter, E.; Shlykov, S. A.; Phien, T. D.; Albanov, A. I.

Synthesis of 3-fluoro-3-methyl-3-silatetrahydropyran and its conformational preferences in gas and solution by GED, NMR and theoretical calculations

Tetrahedron, (74): 1859-1867. 2018. 10.1016/j.tet.2018.02.055

Klosener, J.; Wiesemann, M.; Niemann, M.; Neumann, B.; Stammler, H. G.; Hoge, B.  
Synthesis and Reactivity of Donor-Stabilized Bis(pentafluoroethyl)stannylene Sn(C<sub>2</sub>F<sub>5</sub>)<sub>2</sub>(D)(n)  
(D=THF, DMAP, PMe<sub>3</sub>, Sn(C<sub>2</sub>F<sub>5</sub>)<sub>3</sub> (-))  
Chemistry-a European Journal, (24): 4412-4422. 2018. 10.1002/chem.201705770

Klyne, J.; Bouchet, A.; Ishiuchi, S.; Fujii, M.; Dopfer, O.  
Cation-Size-Dependent Conformational Locking of Glutamic Acid by Alkali Ions: Infrared  
Photodissociation Spectroscopy of Cryogenic Ions  
Journal of Physical Chemistry B, (122): 2295-2306. 2018. 10.1021/acs.jpcb.7b12601

Klyne, J.; Dopfer, O.  
Protonation and Sequential Microsolvation of 5-Hydroxyindole: Infrared Photodissociation  
Spectra of 5H1H(+)-L-n with L = Ar and N-2 (n <= 3)  
Journal of Physical Chemistry B, (122): 10700-10713. 2018. 10.1021/acs.jpcb.8b09023

Klyne, J.; Miyazaki, M.; Fujii, M.; Dopfer, O.  
Sequential microhydration of cationic 5-hydroxyindole (5HI(+)): infrared photodissociation  
spectra of 5HI(+)-W-n clusters (W = H<sub>2</sub>O, n <= 4)  
Physical Chemistry Chemical Physics, (20): 3092-3108. 2018. 10.1039/c7cp06132c

Knighton, R. C.; Emerson-King, J.; Rourke, J. P.; Ohlin, C. A.; Chaplin, A. B.  
Solution, Solid-State, and Computational Analysis of Agostic Interactions in a Coherent Set of  
Low-Coordinate Rhodium(III) and Iridium(III) Complexes  
Chemistry-a European Journal, (24): 4927-4938. 2018. 10.1002/chem.201705990

Ko, Y. J.; Choi, K.; Lee, S.; Jung, K. W.; Hong, S.; Mizuseki, H.; Choi, J. W.; Lee, W. S.  
Strong chromate-adsorbent based on pyrrolic nitrogen structure: An experimental and  
theoretical study on the adsorption mechanism  
Water Research, (145): 287-296. 2018. 10.1016/j.watres.2018.08.033

Kobera, L.; Czernek, J.; Abbrent, S.; Mackova, H.; Pavlovec, L.; Rohlicek, J.; Brus, J.  
The Nature of Chemical Bonding in Lewis Adducts as Reflected by Al-27 NMR Quadrupolar  
Coupling Constant: Combined Solid-State NMR and Quantum Chemical Approach  
Inorganic Chemistry, (57): 7428-7437. 2018. 10.1021/acs.inorgchem.8b01009

Koby, R. F.; Hanusa, T. P.  
Dispersion and distortion in heavy group 2 and lanthanide decamethylmetallocenes: The  
(C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>(Sr,Sm) connection  
Journal of Organometallic Chemistry, (857): 145-151. 2018. 10.1016/j.jorgchem.2017.11.007

Kocasoy, V.; Dedeoglu, B.; Demir-Ordu, O.; Aviyente, V.  
Influence of odd-even effect and intermolecular interactions in 2D molecular layers of bisamide  
organogelators

RSC Advances, (8): 35195-35204. 2018. 10.1039/c8ra06224b

Kochem, A.; Faure, B.; Bertaina, S.; Riviere, E.; Giorgi, M.; Reglier, M.; Orio, M.; Simaan, A. J.  
Magneto-Structural and Computational Study of a Tetranuclear Copper Complex Displaying  
Carbonyl-pi Interactions  
European Journal of Inorganic Chemistry: 5039-5046. 2018. 10.1002/ejic.201801032

Koehle, M.; Zhang, Z. Q.; Goulas, K. A.; Caratzoulas, S.; Vlachos, D. G.; Lobo, R. F.  
Acylation of methylfuran with Bronsted and Lewis acid zeolites  
Applied Catalysis a-General, (564): 90-101. 2018. 10.1016/j.apcata.2018.06.005

Komeiji, Y.; Okiyama, Y.; Mochizuki, Y.; Fukuzawa, K.  
Interaction between a Single-Stranded DNA and a Binding Protein Viewed by the Fragment  
Molecular Orbital Method  
Bulletin of the Chemical Society of Japan, (91): 1596-1605. 2018. 10.1246/bcsj.20180150

Komiya, N.; Hosokawa, T.; Adachi, J.; Inoue, R.; Kawamorita, S.; Naota, T.  
Regiospecific Remote Pt-H Interactions in Oligomethylene-Vaulted (N C N)-Pincer Pt-II  
Complexes  
European Journal of Inorganic Chemistry: 4771-4778. 2018. 10.1002/ejic.201800927

Komrovsky, F.; Sperandeo, N. R.; Vera, D. M. A.; Caira, M. R.; Mazzieri, M. R.  
X-ray, DFT, FTIR and thermal study of the antimicrobial N-benzenesulfonyl-1H-1,2,3-  
benzotriazole  
Journal of Molecular Structure, (1164): 200-208. 2018. 10.1016/j.molstruc.2018.03.012

Konarev, D. V.; Kuzmin, A. V.; Nakano, Y.; Khasanov, S. S.; Otsuka, A.; Yamochi, H.; Kitagawa, H.;  
Lyubovskaya, R. N.  
Synthesis and properties of N-methylimidazole solvates of vanadium(II), chromium(II) and  
iron(II) phthalocyanines. Strong NIR absorption in V-II(MeIm)<sub>2</sub>(Pc<sub>2</sub>-)  
Dalton Transactions, (47): 4661-4671. 2018. 10.1039/c8dt00459e

Kong, X. H.; Wu, Q. Y.; Lan, J. H.; Wang, C. Z.; Chai, Z. F.; Nie, C. M.; Shi, W. Q.  
Theoretical Insights into Preorganized Pyridylpyrazole-Based Ligands toward the Separation of  
Am(III)/Eu(III)  
Inorganic Chemistry, (57): 14810-14820. 2018. 10.1021/acsinorgchem.8b02550

Korenkova, M.; Kremlacek, V.; Erben, M.; Jirasko, R.; De Proft, F.; Turek, J.; Jambor, R.; Ruzicka, A.;  
Cisarova, I.; Dostal, L.  
Heavier pnictinidene gold(I) complexes  
Dalton Transactions, (47): 14503-14514. 2018. 10.1039/c8dt03022g

Kornweitz, H.; Meyerstein, D.

Mechanisms of Reduction of M(H<sub>2</sub>O)(k)(n+) To Form M degrees-Nano-Particles in Aqueous Solutions Differs from That Commonly Assumed: The Reduction of Ag(H<sub>2</sub>O)(2)(+) by H-2  
Journal of Physical Chemistry C, (122): 25043-25050. 2018. 10.1021/acs.jpcc.8b07331

Kosai, T.; Iwamoto, T.

Cleavage of Two Hydrogen Molecules by Boryldisilenes  
Chemistry-a European Journal, (24): 7774-7780. 2018. 10.1002/chem.201801286

Kosanovich, A. J.; Komatsu, C. H.; Bhuvanesh, N.; Perez, L. M.; Ozerov, O. V.

Dearomatization of the PCP Pincer Ligand in a Re-V Oxo Complex  
Chemistry-a European Journal, (24): 13754-13757. 2018. 10.1002/chem.201802589

Koubsky, T.; Lustinec, J.

Application of quantum mechanical simulations for studying the radiolytic stability of prospective extractants in the nuclear fuel cycle  
Journal of Radioanalytical and Nuclear Chemistry, (318): 2407-2413. 2018. 10.1007/s10967-018-6225-2

Kour, M.; Gupta, R.; Bansal, R. K.

Tandem Cope-rearrangement and 2+2 cycloaddition of cis-1,2-diethynylcyclopropane and its mono-hetero analogues: A DFT investigation  
Computational and Theoretical Chemistry, (1123): 142-148. 2018.  
10.1016/j.comptc.2017.12.001

Kovacs, A.

Coordination of N-2 ligands to lanthanum: the complexes La (N-2)(1-8)  
Structural Chemistry, (29): 1825-1837. 2018. 10.1007/s11224-018-1177-2

Kovacs, A.; Dau, P. D.; Marcalo, J.; Gibson, J. K.

Pentavalent Curium, Berkelium, and Californium in Nitrate Complexes: Extending Actinide Chemistry and Oxidation States

Inorganic Chemistry, (57): 9453-9467. 2018. 10.1021/acs.inorgchem.8b01450

Kozytskiy, A. V.; Panasyuk, Y. V.; Mishura, A. M.

Photocatalytic Monofluorination of Unactivated C(sp<sup>3</sup>)-H Bonds by N-Fluorobenzenesulfimide Involving the Decatungstate Anion and the Effect of Water Additives on These Reactions  
Theoretical and Experimental Chemistry, (54): 322-330. 2018. 10.1007/s11237-018-9577-3

Krebs, K. M.; Freitag, S.; Maudrich, J. J.; Schubert, H.; Sirsch, P.; Wesemann, L.

Coordination chemistry of stannylene-based Lewis pairs - insertion into M-Cl and M-C bonds. From base stabilized stanlenes to bidentate ligands  
Dalton Transactions, (47): 83-95. 2018. 10.1039/c7dt04044j

Kremlack, V.; Hyvl, J.; Yoshida, W. Y.; Ruzicka, A.; Rheingold, A. L.; Turek, J.; Hughes, R. P.; Dostal, L.; Cain, M. F.

Heterocycles Derived from Generating Monovalent Pnictogens within NCN Pincers and Bidentate NC Chelates: Hypervalency versus Bell-Clappers versus Static Aromatics  
Organometallics, (37): 2481-2490. 2018. 10.1021/acs.organomet.8b00290

Kremleva, A.; Rosch, N.

Modeling the Effect of the Electrolyte on Standard Reduction Potentials of Polyoxometalates  
Journal of Physical Chemistry C, (122): 18545-18553. 2018. 10.1021/acs.jpcc.8b05426

Krestyaninov, M. A.; Odintsova, E. G.; Kolker, A. M.; Kiselev, M. G.

The structure of water - Acetamide hydrogen bonded complexes. Quantum chemical analysis  
Journal of Molecular Liquids, (264): 343-351. 2018. 10.1016/j.molliq.2018.05.070

Kroeger, A. A.; Karton, A.

A Computational Investigation of the Uncatalysed and Water-Catalysed Acyl Rearrangements in  
Ingenol Esters  
Australian Journal of Chemistry, (71): 212-221. 2018. 10.1071/ch17501

Kruger, J.; Ganesamoorthy, C.; John, L.; Wolper, C.; Schulz, S.

A General Pathway for the Synthesis of Gallastibenes containing Ga=Sb Double Bonds  
Chemistry-a European Journal, (24): 9157-9164. 2018. 10.1002/chem.201801813

Kulinich, A. V.; Ishchenko, A. A.; Bondarev, S. L.; Knyukshto, V. N.

Low-Temperature Effect on the Electronic Structure and Spectral-Fluorescent Properties of  
Highly Dipolar Merocyanines

Journal of Physical Chemistry A, (122): 9645-9652. 2018. 10.1021/acs.jpca.8b09522

Kumar, N. V. S.

Surface enhanced Raman scattering of neutral and zwitterionic alpha- and beta-Proline  
monomers adsorbed on Au-3 cluster: A DFT study

Vibrational Spectroscopy, (98): 15-21. 2018. 10.1016/j.vibspec.2018.06.008

Kumar, R.; Karthick, T.; Tandon, P.; Agarwal, P.; Menezes, A. P.; Jayarama, A.

Structural and vibrational characteristics of a non-linear optical material 3-(4-nitrophenyl)-1-(pyridine-3-yl) prop-2-en-1-one probed by quantum chemical computation and spectroscopic  
techniques

Journal of Molecular Structure, (1164): 180-190. 2018. 10.1016/j.molstruc.2018.03.060

Kumar, R.; Kim, H.; Singh, G.

Experimental and theoretical investigations of a newly synthesized azomethine compound as  
inhibitor for mild steel corrosion in aggressive media: A comprehensive study

Journal of Molecular Liquids, (259): 199-208. 2018. 10.1016/j.molliq.2018.02.123

Kumar, R.; Kim, H.; Umapathi, R.; Yadav, O. S.; Singh, G.

Comprehensive adsorption characteristics of a newly synthesized and sustainable anti-corrosion catalyst on mild steel surface exposed to a highly corrosive electrolytic solution

Journal of Molecular Liquids, (268): 37-48. 2018. 10.1016/j.molliq.2018.06.114

Kumar, R. S.; Almansour, A. I.; Arumugam, N.; Soliman, S. M.; Kumar, R. R.; Altaf, M.; Ghabbour, H. A.; Krishnamoorthy, B. S.

Stereoselective green synthesis and molecular structures of highly functionalized spirooxindole-pyrrolidine hybrids - A combined experimental and theoretical investigation

Journal of Molecular Structure, (1152): 266-275. 2018. 10.1016/j.molstruc.2017.09.073

Kumar, R. S.; Kumar, S. K. A.; Vijayakrishna, K.; Sivaramakrishna, A.; Rao, C.; Sivaraman, N.; Sahoo, S. K.

Development of the Smartphone-Assisted Colorimetric Detection of Thorium by Using New Schiff's Base and Its Applications to Real Time Samples

Inorganic Chemistry, (57): 15270-15279. 2018. 10.1021/acs.inorgchem.8b02564

Kumar, Y.; Bedi, P. M. S.; Singh, P.; Adeniyi, A. A.; Singh-Pillay, A.; Singh, P.; Bhargava, G.

2+2 Cycloadditions of Sorbyl Tosylate with Imines/1-Azadienes: A One-Pot Domino Approach for alpha-Alkylidene-beta-lactams and Their Computational Studies and Antimicrobial Evaluation

Chemistryselect, (3): 9484-9492. 2018. 10.1002/slct.201801605

Kumar, Y.; Kumar, S.; Mandal, K.; Mukhopadhyay, P.

Isolation of Tetracyano-Naphthalenediimide and Its Stable Planar Radical Anion

Angewandte Chemie-International Edition, (57): 16318-16322. 2018. 10.1002/anie.201807836

Kumarasamy, J.; Camarada, M. B.; Venkatraman, D.; Ju, H. X.; Dey, R. S.; Wen, Y. P.

One-step coelectrodeposition-assisted layer-by-layer assembly of gold nanoparticles and reduced graphene oxide and its self-healing three-dimensional nanohybrid for an ultrasensitive DNA sensor

Nanoscale, (10): 1196-1206. 2018. 10.1039/c7nr06952a

Kura, C.; Fujimoto, S.; Kunisada, Y.; Kowalski, D.; Tsuji, E.; Zhu, C.; Habazaki, H.; Aoki, Y.

Enhanced hydrogen permeability of hafnium nitride nanocrystalline membranes by interfacial hydride conduction

Journal of Materials Chemistry A, (6): 2730-2741. 2018. 10.1039/c7ta10253d

Kuruvilla, T. K.; Prasana, J. C.; Muthu, S.; George, J.

Vibrational spectroscopic (FT-IR, FT-Raman) and quantum mechanical study of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno 3,2-f 1,2,4 triazolo 4,3-a 1,4 diazepine

Journal of Molecular Structure, (1157): 519-529. 2018. 10.1016/j.molstruc.2018.01.001

Kuruvilla, T. K.; Prasana, J. C.; Muthu, S.; George, J.; Mathew, S. A.

Quantum mechanical and spectroscopic (FT-IR, FT -Raman) study, NBO analysis, HOMO-LUMO, first order hyperpolarizability and molecular docking study of methyl (3R)-3-(2-methylphenoxy)-3-phenylpropylamine by density functional method

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (188): 382-393. 2018.  
10.1016/j.saa.2017.07.029

Kusama, H.

Comparative study on the interactions of sulfide and iodine mediators with a dye in p-type dye-sensitized solar cells

Journal of Photochemistry and Photobiology a-Chemistry, (365): 110-118. 2018.  
10.1016/j.jphotochem.2018.07.041

Kusama, H.

Interaction between dyes and iodide mediators in p-type dye-sensitized solar cells

Journal of Photochemistry and Photobiology a-Chemistry, (357): 60-71. 2018.  
10.1016/j.jphotochem.2018.02.024

Kuwata, K. T.; Luu, L. N.; Weberg, A. B.; Huang, K.; Parsons, A. J.; Peebles, L. A.; Rackstraw, N. B.; Kim, M. J.

Quantum Chemical and Statistical Rate Theory Studies of the Vinyl Hydroperoxides Formed in trans-2-Butene and 2,3-Dimethyl-2-butene Ozonolysis

Journal of Physical Chemistry A, (122): 2485-2502. 2018. 10.1021/acs.jpca.8b00287

Kwan, E. E.; Zeng, Y. W.; Besser, H. A.; Jacobsen, E. N.

Concerted nucleophilic aromatic substitutions

Nature Chemistry, (10): 917-923. 2018. 10.1038/s41557-018-0079-7

La Penna, G.; Li, M. S.

Towards High-Throughput Modelling of Copper Reactivity Induced by Structural Disorder in Amyloid Peptides

Chemistry-a European Journal, (24): 5259-5270. 2018. 10.1002/chem.201704654

La Porte, N. T.; Martinez, J. F.; Chaudhuri, S.; Hedstrom, S.; Batista, V. S.; Wasielewski, M. R.

Photoexcited radical anion super-reductants for solar fuels catalysis

Coordination Chemistry Reviews, (361): 98-119. 2018. 10.1016/j.ccr.2018.01.018

LaFortune, J. H. W.; Szkop, K. M.; Farinha, F. E.; Johnstone, T. C.; Postle, S.; Stephan, D. W.

Probing steric influences on electrophilic phosphonium cations: a comparison of (3,5-(CF<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>)(3)PF (+) and (C<sub>6</sub>F<sub>5</sub>)(3)PF

Dalton Transactions, (47): 11411-11419. 2018. 10.1039/c8dt02594k

Lagodzinskaya, G. V.; Laptinskaya, T. V.; Kazakov, A. I.

Supramolecular structuring of aqueous solutions of strong acids: manifestations in light scattering, NMR, and oxidation kinetics. Does liquid have a drop-like nature? 1. Nitric acid

Russian Chemical Bulletin, (67): 1838-1850. 2018. 10.1007/s11172-018-2297-y

Lahm, M. E.; Hoobler, P. R.; Turney, J. M.; Peterson, K. A.; Schaefer, H. F.

The bismuth tetramer Bi-4: the v(3) key to experimental observation

Physical Chemistry Chemical Physics, (20): 21881-21889. 2018. 10.1039/c8cp03529f

Lam, E.; Coperet, C.

Understanding Trends in Al-27 Chemical Shifts and Quadrupolar Coupling Constants in Chloroalkyl Aluminum AlCl<sub>x</sub>(Me)(3-x) (n=1 or 2) Compounds

Helvetica Chimica Acta, (101) 2018. 10.1002/hlca.201800120

Lamm, J. H.; Vishnevskiy, Y. V.; Ziemann, E.; Neumann, B.; Stammler, H. G.; Mitzel, N. W.

Regiochemical Control in Triptycene Formation-An Exercise in Subtle Balancing Multiple Factors Chemistryopen, (7): 111-114. 2018. 10.1002/open.201700196

Lan, J. H.; Wu, Q. Y.; Wang, C. Z.; Chai, Z. F.; Shi, W. Q.

Influence of complexing species on the extraction of trivalent actinides from lanthanides with CyMe<sub>4</sub>-BTBP: a theoretical study

Journal of Radioanalytical and Nuclear Chemistry, (318): 1453-1463. 2018. 10.1007/s10967-018-6263-9

Lan, Z. Z.; Sharada, S. M.

Computational strategies to probe CH activation in dioxo-dicopper complexes

Physical Chemistry Chemical Physics, (20): 25602-25614. 2018. 10.1039/c8cp05096a

Landman, M.; van Rensburg, A. J.; van Rooyen, P. H.; Conradie, M. M.; Conradie, J.

Triphenylstibine-substituted Fischer carbene complexes of tungsten(0): synthesis, structure, DFT and electrochemistry

New Journal of Chemistry, (42): 7301-7313. 2018. 10.1039/c8nj01008k

Larranaga, O.; Miranda, J. I.; Cossio, F. P.; de Cozar, A.

Alkaloids Reactivity: DFT Analysis of Selective Demethylation Reactions

Journal of Organic Chemistry, (83): 15101-15109. 2018. 10.1021/acs.joc.8b02364

Laschuk, N. O.; Ebralidze, II; Poisson, J.; Egan, J. G.; Quaranta, S.; Allan, J. T. S.; Cusden, H.; Gaspari, F.; Naumkin, F. Y.; Easton, E. B.; Zenkina, O. V.

Ligand Impact on Monolayer Electrochromic Material Properties

ACS Applied Materials & Interfaces, (10): 35334-35343. 2018. 10.1021/acsami.8b10666

Latypov, S. K.; Ganushevich, Y. S.; Kondrashova, S. A.; Kharlamov, S. V.; Milyukov, V. A.; Sinyashin, O. G.

Structural Diversity and Dynamics of Nickel Complexes with Ambidentate Phosphorus

Heterocycles

Organometallics, (37): 2348-2357. 2018. 10.1021/acs.organomet.8b00319

Le Donne, A.; Bodo, E.

Isomerization patterns and proton transfer in ionic liquids constituents as probed by ab-initio computation

Journal of Molecular Liquids, (249): 1075-1082. 2018. 10.1016/j.molliq.2017.11.152

Lease, N.; Pelczar, E. M.; Zhou, T.; Malakar, S.; Emge, T. J.; Hasanayn, F.; Krogh-Jespersen, K.; Goldman, A. S.

PNP-Pincer Complexes of Osmium: Comparison with Isoelectronic (PCP)Ir and (PNP)Ir+ Units  
Organometallics, (37): 314-326. 2018. 10.1021/acs.organomet.7b00738

Lechuga-Islas, V.; Tlahuext, H.; Falcon-Leon, M. P.; Sanchez-De Jesus, F.; Moo-Puc, R. E.; Chale-Dzul, J. B.; Tapia-Benavides, A. R.; Tlahuextl, M.

Regulating Noncovalent Interactions in Amino-Amide-Copper Complexes  
European Journal of Inorganic Chemistry: 1419-1426. 2018. 10.1002/ejic.201701332

Lee, C. F.; Diaz, D. B.; Holownia, A.; Kaldas, S. J.; Liew, S. K.; Garrett, G. E.; Dudding, T.; Yudin, A. K.

Amine hemilability enables boron to mechanistically resemble either hydride or proton  
Nature Chemistry, (10): 1062-1070. 2018. 10.1038/s41557-018-0097-5

Lee, K. L. K.; Quinn, M. S.; Kolmann, S. J.; Kable, S. H.; Jordan, M. J. T.

Zero-point energy conservation in classical trajectory simulations: Application to H<sub>2</sub>CO  
Journal of Chemical Physics, (148) 2018. 10.1063/1.5023508

Lee, V. Y.; Kawai, M.; Gapurenko, O. A.; Minkin, V. I.; Gornitzka, H.; Sekiguchi, A.

Arsagermene, a compound with an -As=Ge(sic) double bond  
Chemical Communications, (54): 10947-10949. 2018. 10.1039/c8cc05630g

Leenaraj, D. R.; Joe, I. H.

Influence of stereoelectronic effects on the non-opioid analgesics gaboxadol and gaboxadol hydrochloride: Spectral and DFT study

Journal of Physics and Chemistry of Solids, (116): 194-202. 2018. 10.1016/j.jpcs.2018.01.030

Leroy, C.; Schuster, J. K.; Schaefer, T.; Muller-Buschbaum, K.; Braunschweig, H.; Bryce, D. L.

Linear dicoordinate beryllium: a Be-9 solid-state NMR study of a discrete zero-valent s-block beryllium complex

Canadian Journal of Chemistry, (96): 646-652. 2018. 10.1139/cjc-2017-0704

Less, R. J.; Hanf, S.; Garcia-Rodriguez, R.; Bond, A. D.; Wright, D. S.

A HN(BH=NH)(2) (2-) Dianion, Isoelectronic with a beta-Diketiminate  
Organometallics, (37): 628-631. 2018. 10.1021/acs.organomet.7b00436

Levandowski, B. J.; Hamlin, T. A.; Helgeson, R. C.; Bickelhaupt, F. M.; Houk, K. N.

Origins of the Endo and Exo Selectivities in Cyclopropenone, Iminocyclopropene, and Triafulvene Diels-Alder Cycloadditions

Journal of Organic Chemistry, (83): 3164-3170. 2018. 10.1021/acs.joc.8b00025

Levandowski, B. J.; Herath, D.; Gallup, N. M.; Houk, K. N.

Origin of pi-Facial Stereoselectivity in Thiophene 1-Oxide Cycloadditions

Journal of Organic Chemistry, (83): 2611-2616. 2018. 10.1021/acs.joc.7b03016

Levi, E.; Aurbach, D.; Gatti, C.

Do the basic crystal chemistry principles agree with a plethora of recent quantum chemistry data?

lucrj, (5): 542-547. 2018. 10.1107/s2052252518008254

Li, C. C.; Lu, D. M.; Wu, C.

Designing tri-branched multiple-site SO<sub>2</sub> capture materials

Physical Chemistry Chemical Physics, (20): 16704-16711. 2018. 10.1039/c8cp01285g

Li, C. C.; Lu, D. M.; Wu, C.

The role of cations in the interactions between anionic N-heterocycles and SO<sub>2</sub>

Scientific Reports, (8) 2018. 10.1038/s41598-018-25432-6

Li, D. J.; Han, Y.; Li, H. J.; Zhang, P.; Kang, Q.; Li, Z. H.; Shen, D. Z.

The influence of isolated and penta-hydrated Zn<sup>2+</sup> on some of the intramolecular proton-transfer processes of thymine: a quantum chemical study

RSC Advances, (8): 11021-11026. 2018. 10.1039/c7ra13750h

Li, D. J.; Han, Y.; Li, H. J.; Zhang, P.; Kang, Q.; Shen, D. Z.

Do the fragments from decomposed ZIF-8 greatly affect some of the intramolecular proton-transfer of thymine? A quantum chemical study

RSC Advances, (8): 27227-27234. 2018. 10.1039/c8ra03817a

Li, D. J.; Li, H.; Danilov, D.; Gao, L.; Zhou, J.; Eichel, R. A.; Yang, Y.; Notten, P. H. L.

Temperature-dependent cycling performance and ageing mechanisms of C-

6/LiNi1/3Mn1/3Co1/3O2 batteries

Journal of Power Sources, (396): 444-452. 2018. 10.1016/j.jpowsour.2018.06.035

Li, D. Z.; Feng, L. Y.; Zhang, L. J.; Pei, L.; Tian, W. J.; Li, P. F.; Zhai, H. J.

Planar Tricyclic B<sub>8</sub>O<sub>8</sub> and B<sub>8</sub>O<sub>8</sub>- Clusters: Boron Oxide Analogues of s-Indacene C<sub>12</sub>H<sub>8</sub>

Journal of Physical Chemistry A, (122): 2297-2306. 2018. 10.1021/acs.jpca.7b12479

Li, G. F.; Chen, Y. J.; Qiao, Y. J.; Lu, Y. F.; Zhou, G.

Charge Transfer Switching in Donor Acceptor Systems Based on BN-Fused Naphthalimides

Journal of Organic Chemistry, (83): 5577-5587. 2018. 10.1021/acs.joc.8b00597

Li, H.; Wang, X. Y.; Tian, G.; Liu, Y. J.

Insights into the dioxygen activation and catalytic mechanism of the nickel-containing quercetinase

Catalysis Science & Technology, (8): 2340-2351. 2018. 10.1039/c8cy00187a

Li, H.; Wu, B. T.; Wang, J. H.; Wang, F. M.; Zhang, X. B.; Wang, G.; Li, H. C.

Efficient and stable Ru(III)-choline chloride catalyst system with low Ru content for non-mercury acetylene hydrochlorination

Chinese Journal of Catalysis, (39): 1770-1781. 2018. 10.1016/s1872-2067(18)63121-3

Li, H. F.; Goncalves, T. P.; Hu, J. S.; Zhao, Q. Y.; Gong, D. R.; Lai, Z. P.; Wang, Z. X.; Zheng, J. R.; Huang, K. W.

A Pseudodearomatized (PNP)-P-3<sup>\*</sup>Ni-H Complex as a Ligand and sigma-Nucleophilic Catalyst  
Journal of Organic Chemistry, (83): 14969-14977. 2018. 10.1021/acs.joc.8b02205

Li, H. P.; Li, Y. J.; Sun, L. H.; Xun, S. H.; Jiang, W.; Zhang, M.; Zhu, W. S.; Li, H. M.

H<sub>2</sub>O<sub>2</sub> decomposition mechanism and its oxidative desulfurization activity on hexagonal boron nitride monolayer: A density functional theory study

Journal of Molecular Graphics & Modelling, (84): 166-173. 2018. 10.1016/j.jmgm.2018.07.002

Li, H. R.; Liu, H.; Lu, X. Q.; Zan, W. Y.; Tian, X. X.; Lu, H. G.; Wu, Y. B.; Mu, Y. W.; Li, S. D.

Cage-like Ta@B-n(q) complexes (n=23-28, q =-1-+3) in 18-electron configurations with the highest coordination number of twenty-eight

Nanoscale, (10): 7451-7456. 2018. 10.1039/c8nr01087k

Li, J. B.; Tadakamalla, D.; Rogachev, A. Y.

Modulating stability of functionalized fullerene cations R-C-60 (+) with the nature of R-group  
Journal of Computational Chemistry, (39): 2385-2396. 2018. 10.1002/jcc.25579

Li, J. F.; Zhao, R. F.; Chai, X. T.; Zhou, F. Q.; Li, C. C.; Li, J. L.; Yin, B.

Why do higher VDEs of superhalogen not ensure improved stabilities of the noble gas hydrides promoted by them? A high-level ab initio case study

Journal of Chemical Physics, (149) 2018. 10.1063/1.5038191

Li, J. Q.; Geng, S.; Liu, B. G.; Wang, H. B.; Liang, G. Z.

Self-assembled mechanism of hydrophobic amino acids and beta-cyclodextrin based on experimental and computational methods

Food Research International, (112): 136-142. 2018. 10.1016/j.foodres.2018.06.017

Li, L. F.; Lei, M.; Liu, L.; Xie, Y. M.; Schaefer, H. F.

Metal-Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst

Inorganic Chemistry, (57): 8778-8787. 2018. 10.1021/acs.inorgchem.8b00563

Li, L. F.; Lei, M.; Xie, Y. M.; Weinhold, F.; Schaefer, H. F.

Quantitative Theoretical Predictions and Qualitative Bonding Analysis of the Divinylborinium System and Its Al, Ga, In, and Tl Congeners

Inorganic Chemistry, (57): 7851-7859. 2018. 10.1021/acs.inorgchem.8b00968

Li, L. F.; Zhu, H. J.; Liu, L.; Song, D. T.; Lei, M.

A Hydride-Shuttle Mechanism for the Catalytic Hydroboration of CO<sub>2</sub>

Inorganic Chemistry, (57): 3054-3060. 2018. 10.1021/acs.inorgchem.7b02887

Li, L. W.; Wu, C. J.; Li, Z.; Xie, W. B.; Guo, X.; Zhou, Z. X.; Sun, T. M.

Conformational and characterization of benidipine hydrochloride polymorphs: Spectroscopic and computational modeling investigations

Journal of Molecular Structure, (1164): 493-500. 2018. 10.1016/j.molstruc.2018.03.103

Li, L. W.; Zhou, Y. N.; Wang, Z. J.; Wu, C. J.; Li, Z.; Sun, C. S.; Sun, T. M.

Theoretical studies on the mechanism of sugammadex for the reversal of aminosteroid-induced neuromuscular blockade

Journal of Molecular Liquids, (265): 450-456. 2018. 10.1016/j.molliq.2018.06.033

Li, P. J.; Li, L. F.; Yue, X.; Wang, Q. Y.; Pu, M.; Yang, Z. Y.; Lei, M.

1,2 addition or cycloaddition of allenes by a dihafnium mu-Nitrido complex? A DFT study

Journal of Organometallic Chemistry, (874): 101-105. 2018. 10.1016/j.jorganchem.2018.08.015

Li, Q. Z.; Zheng, J. J.; He, L.; Nagase, S.; Zhao, X.

La-La bonded dimetallocfullerenes La-2@C-2n (-): species for stabilizing C-2n (2n=92-96) besides La<sub>2</sub>C<sub>2</sub>@C-2n

Physical Chemistry Chemical Physics, (20): 14671-14678. 2018. 10.1039/c8cp01371c

Li, R.; You, X. R.; Wang, K.; Zhai, H. J.

Nature of Bonding in Bowl-Like B-36 Cluster Revisited: Concentric (6+18) Double Aromaticity and Reason for the Preference of a Hexagonal Hole in a Central Location

Chemistry-an Asian Journal, (13): 1148-1156. 2018. 10.1002/asia.201800174

Li, W. L.; Lu, J. B.; Zhao, L. L.; Ponec, R.; Cooper, D. L.; Li, J.; Frenking, G.

Electronic Structure and Bonding Situation in M<sub>2</sub>O<sub>2</sub> (M = Be, Mg, Ca) Rhombic Clusters

Journal of Physical Chemistry A, (122): 2816-2822. 2018. 10.1021/acs.jpca.8b01335

Li, W. X.; Spada, L.; Tasinato, N.; Rampino, S.; Evangelisti, L.; Gualandi, A.; Cozzi, P. G.; Melandri, S.; Barone, V.; Puzzarini, C.

Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions

Angewandte Chemie-International Edition, (57): 13853-13857. 2018. 10.1002/anie.201807751

Li, X. J.

Design of novel graphdiyne-based materials with large second-order nonlinear optical properties

Journal of Materials Chemistry C, (6): 7576-7583. 2018. 10.1039/c8tc02146e

Li, X. M.; Pan, Y. R.; Liu, B.; Zhou, S.; Chang, Y. F.

Syntheses, Crystal Structures and Theoretical Calculations of Cadmium/Zinc Supramolecular Coordination Compounds

Chinese Journal of Inorganic Chemistry, (34): 1923-1928. 2018. 10.11862/cjic.2018.225

Li, X. M.; Wang, Z. T.; Pan, Y. R.; Wang, Q. W.; Liu, B.

Synthesis, Crystal Structure and Theoretical Calculations of Two Zinc, Cobalt Coordination Polymers with 5-Nitroisophthalic Acid and 1,4-Bis(1H-benzimidazolyl)butane Ligands

Journal of Inorganic and Organometallic Polymers and Materials, (28): 258-267. 2018.

10.1007/s10904-017-0738-y

Li, X. Y.

Covalent character and electric field dependence of H-2-AgX (X = F - I)

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3703-y

Li, X. Y.; Cao, X.

On the covalence in H-2 - AuX (X = F-I)

International Journal of Hydrogen Energy, (43): 1709-1717. 2018.

10.1016/j.ijhydene.2017.11.152

Li, Y.; Fu, W. W.; Liang, C. H.

Mechanisms and stereoselectivities of phosphine-catalyzed domino reaction of alpha-benzyl allenolate with 5-phenylmethylene thiazolone: a computational investigation

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-017-2174-z

Li, Y.; Fu, W. W.; Tian, R. X.; Liang, C. H.

Mechanisms and stereoselectivities of phosphine-catalyzed (3+3) cycloaddition reaction between azomethine imine and ynone: A computational study

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25729

Li, Y.; Xu, Z. F.

Competition between tetrel bond and pnicogen bond in complexes of TX3-ZX(2) and NH3

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3732-6

Li, Y.; Zhang, Z. Q.; Liang, C. H.

Understanding the mechanism and stereoselectivity of NHC-catalyzed 3+2 cycloaddition of 3-bromoenals and isatin N-Boc ketimines

Organic & Biomolecular Chemistry, (16): 9251-9258. 2018. 10.1039/c8ob02804d

Li, Y. K.; Zhao, Y. X.; He, S. G.

Selective Conversion of Methane by Rh-1-Doped Aluminum Oxide Cluster Anions RhAl<sub>2</sub>O<sub>4</sub><sup>-</sup>: A Comparison with the Reactivity of PtAl<sub>2</sub>O<sub>4</sub>

Journal of Physical Chemistry A, (122): 3950-3955. 2018. 10.1021/acs.jpca.8b02483

Li, Y. L.; Zou, J. H.; Xiong, X. G.; Xie, H.; Tang, Z. C.; Ge, M.; Zhao, Y. F.; Liu, H. T.

Anion photoelectron spectroscopy and chemical bonding of ThO<sub>2</sub><sup>-</sup> and ThO<sub>3</sub>

Journal of Chemical Physics, (148) 2018. 10.1063/1.5030142

Li, Y. W.; Liu, J. H.; Hou, C.; Shao, Y. X.; Qu, L. B.; Zhao, C. Y.; Ke, Z. F.

Elucidating metal hydride reactivity using late transition metal boryl and borane hydrides:  $2c-2e$  terminal hydride,  $3c-2e$  bridging hydride, and  $3c-4e$  bridging hydride

Catalysis Science & Technology, (8): 3395-3405. 2018. 10.1039/c8cy00766g

Li, Y. Z.; Yuan, D. D.; Wang, Q. C.; Li, W.; Li, S. H.

Accurate prediction of the structure and vibrational spectra of ionic liquid clusters with the generalized energy-based fragmentation approach: critical role of ion-pair-based fragmentation

Physical Chemistry Chemical Physics, (20): 13547-13557. 2018. 10.1039/c8cp00513c

Li, Z.; Li, L. W.; Zheng, Y.; Chen, C.; Sun, T. M.

Diagnostic absolute configuration determination of clavulanate potassium: A comprehensive investigation of chiroptical spectroscopies and theoretical calculations

Journal of Pharmaceutical and Biomedical Analysis, (160): 351-359. 2018.

10.1016/j.jpba.2018.08.010

Li, Z. F.; Yang, X. P.; Li, H. X.; Zuo, G. F.

Phosphorescent Modulation of Metallophilic Clusters and Recognition of Solvents through a Flexible Host-Guest Assembly: A Theoretical Investigation

Nanomaterials, (8) 2018. 10.3390/nano8090685

Li, Z. L.; Li, W. W.; Liu, F.; Wang, X. Y.

Theoretical design on a new double functional device of 2,2-bipyridine-embedded N-(9-pyrenyl methyl)aza-15-crown-5

Journal of Physical Organic Chemistry, (31) 2018. 10.1002/poc.3792

Li, Z. S.; Hou, Y. F.; Li, Y. Q.; Hinz, A.; Chen, X. D.

Biradicaloid and Zwitterion Reactivity of Dicarbondiphosphide Stabilized with N-Heterocyclic Carbenes

Chemistry-a European Journal, (24): 4849-4855. 2018. 10.1002/chem.201705403

Li, Z. Z.; Li, A. Y.

B(4)Rg&ITn&IT2+ (Rg = He similar to Rn, &ITn&IT=1-4): In quest of the potential trapping ability of the aromatic B-4(2+) ring

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25530

Li, Z. Z.; Li, A. Y.

Compounds with Rare Gas-Selenium/Tellurium Bonds: A Theoretical Investigation on FRgLF(n) and FRgLF(n-1)(+)(Rg = Kr-Rn, L = Se and Te, n=1, 3, and 5)

Journal of Physical Chemistry A, (122): 5445-5454. 2018. 10.1021/acs.jpca.7b12834

Liang, J. X.; Su, Q.; Wang, X. E.

Structures and Electronic Properties of Anions XO<sup>-</sup> (X = Li, B, N, F, Na, Al, P, and Cl) from a Computational Study

Chiang Mai Journal of Science, (45): 2409-2421. 2018.

Liang, J. X.; Wang, Y. X.; Liu, L.

Effects of substitutions in the equatorial position on the stabilities of pentacoordinated silicon anions ClSiabcOCl(-) (a, b, c = H, F, Cl) from theoretical investigation

Journal of the Chinese Chemical Society, (65): 1179-1187. 2018. 10.1002/jccs.201700421

Liang, W. Y.; Das, A.; Dong, X.; Cui, Z. H.

Lithium doped tubular structure in LiB<sub>20</sub> and LiB<sub>20</sub><sup>-</sup>: a viable global minimum

Physical Chemistry Chemical Physics, (20): 16202-16208. 2018. 10.1039/c8cp01376d

Liao, J. H.; Kahlal, S.; Liu, Y. C.; Chiang, M. H.; Saillard, J. Y.; Liu, C. W.

Identification of an Eight-Electron Superatomic Cluster and Its Alloy in One Co-crystal Structure

Journal of Cluster Science, (29): 827-835. 2018. 10.1007/s10876-018-1353-y

Liao, K. B.; Liu, W. B.; Niemeyer, Z. L.; Ren, Z.; Bacsa, J.; Musaev, D. G.; Sigman, M. S.; Davies, H. M. L.

Site-Selective Carbene-Induced C-H Functionalization Catalyzed by Dirhodium

Tetrakis(triaryl)cyclopropanecarboxylate) Complexes

ACS Catalysis, (8): 678-682. 2018. 10.1021/acscatal.7b03421

Liljenberg, M.; Stenlid, J. H.; Brinck, T.

Theoretical Investigation into Rate-Determining Factors in Electrophilic Aromatic Halogenation

Journal of Physical Chemistry A, (122): 3270-3279. 2018. 10.1021/acs.jpca.7b10781

Limon, P.; Miralrio, A.; Castro, M.

Adsorption and dissociation of carbon monoxide on iron and iron-carbon clusters: Fe-n+2CO and FenC+2CO, n=4 and 7. A theoretical study

Computational and Theoretical Chemistry, (1129): 37-47. 2018. 10.1016/j.comptc.2018.02.018

Lin, J. L.; Qin, B.; Zhao, G. L.

Effect of solvents on photocatalytic reduction of CO<sub>2</sub> mediated by cobalt complex

Journal of Photochemistry and Photobiology a-Chemistry, (354): 181-186. 2018.

10.1016/j.jphotochem.2017.09.019

Lin, X. H.; Jiang, X. Y.; Wu, W.; Mo, Y. R.

Induction, Resonance, and Secondary Electrostatic Interaction on Hydrogen Bonding in the Association of Amides and Imides

Journal of Organic Chemistry, (83): 13446-13453. 2018. 10.1021/acs.joc.8b02247

Lin, X. H.; Wu, W.; Wiherg, K. B.; Mo, Y. R.

Role of Intramolecular Electron Delocalization in the C-X Bond Strength in CH<sub>4-n</sub>X<sub>n</sub> (n=0-4, X = F, Cl, CN, OCH<sub>3</sub>)

Journal of Physical Chemistry A, (122): 7716-7722. 2018. 10.1021/acs.jpca.8b07427

Lipke, M. C.; Poradowski, M. N.; Raynaud, C.; Eisenstein, O.; Tilley, T. D.

Catalytic Olefin Hydrosilations Mediated by Ruthenium eta(3)-H<sub>2</sub>Si sigma Complexes of Primary and Secondary Silanes

ACS Catalysis, (8): 11513-11523. 2018. 10.1021/acscatal.8b02161

Liu, C. G.; Chu, Y. J.

Activation mechanism of hydrogen peroxide by a divanadium-substituted polyoxometalate gamma-PV<sub>2</sub>W<sub>10</sub>O<sub>38</sub>(mu-OH)(2) (3-): A computational study

Journal of Molecular Graphics & Modelling, (85): 56-67. 2018. 10.1016/j.jmgm.2018.07.009

Liu, C. G.; Sun, C.; Jiang, M. X.; Zhang, Y. T.

Computational study on the catalytic cycle for reduction of NO to N<sub>2</sub> catalyzed by a ruthenium-substituted Keggin-type polyoxometalate

Computational and Theoretical Chemistry, (1140): 104-116. 2018.

10.1016/j.comptc.2018.08.004

Liu, H.; Li, C. B.; Li, G. F.; Li, X. M.; Pan, Y. R.

Syntheses, Crystal Structures and Theoretical Calculation of Cadmium/Lead Supramolecular Coordination Compounds

Chinese Journal of Inorganic Chemistry, (34): 161-169. 2018. 10.11862/cjic.2018.003

Liu, H. C.; Luo, Q. H.; Zhang, S.; Shi, L. D.; Yang, J. L.; Liu, R. G.; Wang, M. L.; Zhu, C. Z.; Xu, J.

New comonomer for polyacrylonitrile-based carbon fiber: Density functional theory study and experimental analysis

Polymer, (153): 369-377. 2018. 10.1016/j.polymer.2018.08.041

Liu, J.; Chen, Q. W.; He, Q. L.; Zhang, Y. J.; Fu, X. Y.; Wang, Y. F.; Zhao, D. H.; Chen, W.; Xu, G. Q.; Wu, K.

Bromine adatom promoted C-H bond activation in terminal alkynes at room temperature on Ag(111)

Physical Chemistry Chemical Physics, (20): 11081-11088. 2018. 10.1039/c7cp07972a

Liu, J. Y.; Li, R. Y.; Li, Y.; Ma, H. D.; Wu, D.

Superalkali Cations with Trivalent Anion MF<sub>63-</sub> (M = Al, Ga, Sc) as Central Core

Journal of Cluster Science, (29): 853-860. 2018. 10.1007/s10876-018-1363-9

- Liu, N.; You, X. R.; Zhai, H. J.  
Chemical Bonding in Transition Metal Nitride Os<sub>3</sub>N<sub>3+</sub> Cluster: 6 pi Inorganic Benzene and delta(2)delta\*(1)delta\*(1) Aromaticity  
ACS Omega, (3): 17083-17091. 2018. 10.1021/acsomega.8b02709
- Liu, P.; Bian, J. H.; Wang, Q.; Huang, F.; Li, D. B.; Wu, Y. B.  
CB<sub>3</sub>E<sub>2</sub>q (q = +/- 1): a family of "hyparene" analogues with a planar pentacoordinate carbon  
Physical Chemistry Chemical Physics, (20): 12642-12649. 2018. 10.1039/c8cp01193a
- Liu, Q. Z.; Li, K.; Lv, G. C.; Li, X.; Peng, Y.; Lin, J. G.; Qiu, L.  
Density functional theory studies on a non-covalent interaction system: hydrogen-bonded dimers of zoledronate  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3826-1
- Liu, S. Y.; Dang, Z. Y.; Liu, D.; Zhang, C. C.; Huang, T.; Yu, A. S.  
Comparative studies of zirconium doping and coating on LiNi(0.6)Co(0.2)Mn(0.2)O<sub>2</sub> cathode material at elevated temperatures  
Journal of Power Sources, (396): 288-296. 2018. 10.1016/j.jpowsour.2018.06.052
- Liu, S. Y.; Rogachev, A. Y.  
Comprehensive Theoretical Study of Interactions between Ag<sup>+</sup> and Polycyclic Aromatic Hydrocarbons  
Chemphyschem, (19): 2579-2588. 2018. 10.1002/cphc.201800297
- Liu, T.; Li, J.; Liu, W. J.; Zhu, Y. D.; Lu, X. H.  
Simple Ligand Modifications to Modulate the Activity of Ruthenium Catalysts for CO<sub>2</sub> Hydrogenation: Trans Influence of Boryl Ligands and Nature of Ru-H Bond  
Acta Physico-Chimica Sinica, (34): 1097-1105. 2018. 10.3866/pku.Whxb201712131
- Liu, X.; Liu, X. R.; Wang, X. F.  
Splitting of Hydrogen Sulfide by Group 14 Elements (Si, Ge, Sn, Pb) in Excess Argon at Cryogenic Temperatures  
Journal of Physical Chemistry A, (122): 7023-7032. 2018. 10.1021/acs.jpca.8b04428
- Liu, Y.; Korn, J. A.; Dang, A.; Turecek, F.  
Hydrogen-Rich Cation Radicals of DNA Dinucleotides: Generation and Structure Elucidation by UV-Vis Action Spectroscopy  
Journal of Physical Chemistry B, (122): 9665-9680. 2018. 10.1021/acs.jpcb.8b07925
- Liu, Y.; Wang, J. F.  
Lewis Acidity and Basicity of Mixed Chlorometallate Ionic Liquids: Investigations from Surface Analysis and Fukui Function  
Molecules, (23) 2018. 10.3390/molecules23102516

- Liu, Y. H.; Yang, Y. Y.; Zhu, R. X.; Liu, C. B.; Zhang, D. J.  
The Dual Role of Gold(I) Complexes in Photosensitizer-Free Visible-Light-Mediated Gold-Catalyzed 1,2-Difunctionalization of Alkynes: A DFT Study  
Chemistry-a European Journal, (24): 14119-14126. 2018. 10.1002/chem.201803075
- Liu, Z. M.; Barigye, S. J.; Shahamat, M.; Labute, P.; Moitessier, N.  
Atom Types Independent Molecular Mechanics Method for Predicting the Conformational Energy of Small Molecules  
Journal of Chemical Information and Modeling, (58): 194-205. 2018. 10.1021/acs.jcim.7b00645
- Loan, H. T. P.; Duc, H. V.; Quang, D. T.; Tat, P. V.; Hiep, D. T.; Nhun, N. T. A.  
Theoretically predicted divalent silicon(0) compounds: Structures and chemical bonding of silylone in molybdenum pentacarbonyl complexes  $\text{Mo}(\text{CO})(5)\text{-Si}(\text{X}\text{Cp}^*)(2)$  ( $\text{X} = \text{B-Tl}$ )  
Computational and Theoretical Chemistry, (1131): 13-24. 2018. 10.1016/j.comptc.2018.03.021
- Lobayan, R. M.; Schmit, M. C. P.  
Conformational and NBO studies of serotonin as a radical scavenger. Changes induced by the OH group  
Journal of Molecular Graphics & Modelling, (80): 224-237. 2018. 10.1016/j.jmgm.2018.01.006
- Lokesh, N.; Seegerer, A.; Hioe, J.; Gschwind, R. M.  
Chemical Exchange Saturation Transfer in Chemical Reactions: A Mechanistic Tool for NMR Detection and Characterization of Transient Intermediates  
Journal of the American Chemical Society, (140): 1855-1862. 2018. 10.1021/jacs.7b12343
- Lopez, S. F.; Meza, M. P.; Hoyos, F. T.  
Study of the nonlinear optical properties of 4-nitroaniline type compounds by density functional theory calculations: Towards new NLO materials  
Computational and Theoretical Chemistry, (1133): 25-32. 2018. 10.1016/j.comptc.2018.04.016
- Lu, C. X.; Tang, Z. G.; Gao, X. X.; Ma, X. M.; Liu, C. B.  
Computer-aided design of magnetic dummy molecularly imprinted polymers for solid-phase extraction of ten phthalates from food prior to their determination by GC-MS/MS  
Microchimica Acta, (185) 2018. 10.1007/s00604-018-2892-5
- Lu, F. F.; Yang, L. H.; Dang, Y. R.; Li, Q. Z.; Li, X. Y.  
Theoretical assessing on the coordination mode and bonding in heteronuclear group-13 dimetallocene  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25461
- Lu, J. S.; Yang, M. C.; Su, M. D.  
Is It Possible To Prepare and Stabilize Triple-Bonded Thallium Antimony Molecules Using Substituents?  
ACS Omega, (3): 10163-10171. 2018. 10.1021/acsomega.8b00643

Lu, J. S.; Yang, M. C.; Su, M. D.

A possible target: triple-bonded indium equivalent to Rantimony molecules with high stability  
New Journal of Chemistry, (42): 6932-6941. 2018. 10.1039/c8nj00549d

Lu, S. J.

Probing the geometric structures and electronic properties of anionic and neutral Pt<sub>3</sub>C<sub>2</sub> clusters by density functional calculations  
Chemical Physics Letters, (694): 70-74. 2018. 10.1016/j.cplett.2018.01.050

Lu, S. J.

Probing the structural evolution and bonding properties of Pt<sub>n</sub>C<sub>2</sub>-/0 (n=1-7) clusters by density functional calculations  
Chemical Physics Letters, (699): 218-222. 2018. 10.1016/j.cplett.2018.03.071

Lu, S. J.

Structures and bonding properties of Pd<sub>n</sub>C<sub>2</sub>-/0 (n=1-7) clusters

Chemical Physics Letters, (705): 65-70. 2018. 10.1016/j.cplett.2018.05.057

Lu, S. J.; Wu, L. S.; Lin, F.

Probing the geometric structures and bonding mechanisms of Cu-I hybrid clusters: Cu<sub>4</sub>I<sub>4</sub>-/0  
Computational and Theoretical Chemistry, (1139): 102-105. 2018.

10.1016/j.comptc.2018.07.012

Lu, S. J.; Xu, X. L.; Cao, G. J.; Xu, H. G.; Zhen, W. J.

Structural evolution and bonding properties of BSin-/0 (n=4-12) clusters: Size-selected anion photoelectron spectroscopy and theoretical calculations

Journal of Chemical Physics, (149) 2018. 10.1063/1.5052559

Lu, S. J.; Xu, X. L.; Cao, G. J.; Xu, H. G.; Zheng, W. J.

Structural Evolution of B<sub>2</sub>Sin-/0 (n=3-12) Clusters: Size-Selected Anion Photoelectron Spectroscopy and Theoretical Calculations

Journal of Physical Chemistry C, (122): 2391-2401. 2018. 10.1021/acs.jpcc.7b10906

Lu, S. J.; Xu, X. L.; Xu, H. G.; Zheng, W. J.

Structural evolution and bonding properties of Au<sub>2</sub>Sin-/0 (n=1-7) clusters: Anion photoelectron spectroscopy and theoretical calculations

Journal of Chemical Physics, (148) 2018. 10.1063/1.5029870

Luo, Q. H.; Li, G.; Xiao, J. P.; Yin, C. H.; He, Y. H.; Wang, M. L.; Ma, C. S.; Zhu, C. Z.; Xu, J.

DFT study on the hydrolysis of metsulfuron-methyl: A sulfonylurea herbicide

Journal of Theoretical & Computational Chemistry, (17) 2018. 10.1142/s0219633618500505

Lutz, P. B.; Bayse, C. A.

Interpreting geometric preferences in -stacking interactions through molecular orbital analysis  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25513

Lv, H. H.; Ren, Z. Q.; Liu, H.; Zhang, G. B.; He, H. P.; Zhang, X. H.; Wang, S. F.  
The turn-off fluorescent sensors based on thioether-linked bisbenzamide for Fe<sup>3+</sup> and Hg<sup>2+</sup>  
Tetrahedron, (74): 1668-1680. 2018. 10.1016/j.tet.2018.02.031

Lv, J.; Yang, L. H.; Sun, Z.; Meng, L. P.; Li, X. Y.  
Nature of non-nuclear (3,-3) pi-attractor and pi-bonding: Theoretical analysis on pi-electron density  
Chemical Physics Letters, (691): 347-350. 2018. 10.1016/j.cplett.2017.11.032

Lv, S.; Bai, F. Y.; Pan, X. M.; Zhao, L.  
Theoretical insight into the role of urea in the hydrolysis reaction of NO<sub>2</sub> as a source of HONO and aerosols  
Environmental Chemistry, (15): 372-385. 2018. 10.1071/en18083

Lyu, Y. J.; Qi, T.; Yang, H. Q.; Hu, C. W.  
Performance of edges on carbon for the catalytic hydroxylation of benzene to phenol  
Catalysis Science & Technology, (8): 176-186. 2018. 10.1039/c7cy01648d

Lyubov, D. M.; Cherkasov, A. V.; Fukin, G. K.; Lyssenko, K. A.; Rychagova, E. A.; Ketkov, S. Y.; Trifonov, A. A.  
Rare-earth metal-mediated PhCu N insertion into N, N-bis(trimethylsilyl) naphthalene-1,8-diamido dianion - a synthetic approach to complexes coordinated by ansa-bridged amido-amidinato ligand  
Dalton Transactions, (47): 438-451. 2018. 10.1039/c7dt03809g

Ma, F. F.; Ding, Z. Z.; Elm, J.; Xie, H. B.; Yu, Q.; Liu, C.; Lo, C.; Fu, Z. Q.; Zhang, L. L.; Chen, J. W.  
Atmospheric Oxidation of Piperazine Initiated by center dot Cl: Unexpected High Nitrosamine Yield  
Environmental Science & Technology, (52): 9801-9809. 2018. 10.1021/acs.est.8b02510

Ma, H. D.; Li, Y.; Liu, J. Y.; Wu, D.  
Characterisation of superalkaline-earth-metal halides, hydroxide and chalcogenides  
Molecular Physics, (116): 1871-1882. 2018. 10.1080/00268976.2018.1459919

Ma, Y.; Zhang, Y.; Chen, C.; Zhang, J. S.; Fan, B. W.; Wang, T. F.; Ren, T. G.; Wang, L.; Zhang, J. L.  
Insight on asym-Pyrazolium Ionic Liquids for Chemical Fixation of CO<sub>2</sub> and Propylene Epoxide into Propylene Carbonate without Organic Solvent and Metal  
Industrial & Engineering Chemistry Research, (57): 13342-13352. 2018.  
10.1021/acs.iecr.8b02318

Ma, Y. P.; Hu, C. C.; Guo, H. X.; Fan, L.; Yang, S. Y.; Sun, W. H.

Structure effect on transition mechanism of UV-visible absorption spectrum in polyimides: A density functional theory study

Polymer, (148): 356-369. 2018. 10.1016/j.polymer.2018.06.049

Machado, N.; Carvalho, B. G.; Soto, C. A. T.; Martin, A. A.; Favero, P. P.

DFT application for chlorin derivatives photosensitizer drugs modeling

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (195): 68-74. 2018.

10.1016/j.saa.2018.01.045

Madhu, D. K.; Madhavan, J.

Quantum chemical analysis of electronic structure and bonding aspects of choline based ionic liquids

Journal of Molecular Liquids, (249): 637-649. 2018. 10.1016/j.molliq.2017.11.080

Mafune, F.; Masuzaki, D.; Nagata, T.

Reduction Site in CenVmOk+ Revealed by Gas Phase Thermal Desorption Spectrometry

Topics in Catalysis, (61): 42-48. 2018. 10.1007/s11244-017-0862-5

Mahjoobizadeh, M.; Takjoo, R.; Farhadipour, A.; Mague, J. T.

Fe(III), Cu(II) and U(VI) binuclear complexes with a new isothiosemicarbazone ligand: Syntheses, characterization, crystal structures, thermal behavior and theoretical investigations

Inorganica Chimica Acta, (482): 643-653. 2018. 10.1016/j.ica.2018.07.011

Mahler, A.; Janesko, B. G.; Moncho, S.; Brothers, E. N.

When Hartree-Fock exchange admixture lowers DFT-predicted barrier heights: Natural bond orbital analyses and implications for catalysis

Journal of Chemical Physics, (148) 2018. 10.1063/1.5032218

Mahmoodi, A.; Panahi, F.; Eshghi, F.; Kimiae, E.

A novel tetra-stilbene-based fluorescent compound: Synthesis, characterization and photophysical properties evaluation

Journal of Luminescence, (199): 165-173. 2018. 10.1016/j.jlumin.2018.03.033

Mahmoud, M. A. M.; El-Demerdash, S. H.; El Gogary, T. M.; El-Nahas, A. M.

Oxidation of Methyl Propanoate by the OH Radical

Russian Journal of Physical Chemistry A, (92): 2476-2484. 2018. 10.1134/s0036024418120294

Mahsoune, A.; Sadik, K.; Belghiti, M. E.; Bahadur, I.; Aboulmouhajir, A.

Toward a Theoretical Understanding of the Corrosion Inhibitive Performance on Iron Surface by Some Macrocyclic Polyether Compounds Containing 1, 3, 4-thiadiazole Entity

International Journal of Electrochemical Science, (13): 8396-8427. 2018. 10.20964/2018.09.13

Maihom, T.; Kaewruang, S.; Phattharasupakun, N.; Chiochan, P.; Limtrakul, J.; Sawangphruk, M.

Lithium Bond Impact on Lithium Polysulfide Adsorption with Functionalized Carbon Fiber Paper Interlayers for Lithium-Sulfur Batteries

Journal of Physical Chemistry C, (122): 7033-7040. 2018. 10.1021/acs.jpcc.7b09392

Maihom, T.; Sawangphruk, M.; Probst, M.; Limtrakul, J.

A computational study of the catalytic aerobic epoxidation of propylene over the coordinatively unsaturated metal-organic framework Fe-3(btc)(2): formation of propylene oxide and competing reactions

Physical Chemistry Chemical Physics, (20): 6726-6734. 2018. 10.1039/c7cp07550b

Maity, A.; Sinha, D.; Rajak, K. K.

Experimental and theoretical studies of structural and photophysical properties of a novel heteroleptic cyclometalated iridium(III) complex with 8-hydroxyquinoline-phenylazo ligand

Journal of Molecular Structure, (1158): 122-132. 2018. 10.1016/j.molstruc.2018.01.006

Maity, B.; Koley, D.

Solvent-Promoted Regio- and Stereoselectivity in Ru-Catalyzed Hydrocarboxylation of Terminal Alkynes: A DFT Study

Chemcatchem, (10): 566-580. 2018. 10.1002/cctc.201701345

Maity, L.; Das Adhikary, S.; Mondal, A.; Kisan, H. K.; Isab, A. A.; Goswami, S.; Dinda, J.

Synthesis, structure, theoretical studies and electrochemistry of Ru(II)-N heterocyclic carbenes  
Inorganica Chimica Acta, (479): 141-147. 2018. 10.1016/j.ica.2018.04.029

Majumder, A.; Ghara, M.; Chattaraj, P. K.

Exohedral complexation of B-39(-) with ECp<sup>\*</sup>+ half-sandwich complexes (E=Si Ge, Sn, Pb): A DFT study

Computational and Theoretical Chemistry, (1140): 49-55. 2018. 10.1016/j.comptc.2018.07.018

Makhlof, M. M.; Radwan, A. S.; Ghazal, B.

Experimental and DFT insights into molecular structure and optical properties of new chalcones as promising photosensitizers towards solar cell applications

Applied Surface Science, (452): 337-351. 2018. 10.1016/j.apsusc.2018.05.007

Malarkodi, H.; Saminathan, M.; Ezhilarasi, R.; Murugan, D.; Ponnuswamy, A.

Molecular Structure, Spectral, Electronic and Thermodynamic, First-Order Hyperpolarizability, NBO and Molecular Docking Studies of Novel Acenaphthylene Pyrrolidine Derivative

Chemistryselect, (3): 11552-11564. 2018. 10.1002/slct.201802535

Malladi, S.; Yarasi, S.; Sastry, G. N.

Exploring the potential of iron to replace ruthenium in photosensitizers: a computational study

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3870-x

Malwal, S. R.; Gao, J.; Hu, X. Y.; Yang, Y. Y.; Liu, W. D.; Huang, J. W.; Ko, T. P.; Li, L. P.; Chen, C. C.; O'Dowd, B.; Khade, R. L.; Zhang, Y.; Zhang, Y. H.; Oldfield, E.; Guo, R. T.  
Catalytic Role of Conserved Asparagine, Glutamine, Serine, and Tyrosine Residues in Isoprenoid Biosynthesis Enzymes

ACS Catalysis, (8): 4299-4312. 2018. 10.1021/acscatal.8600543

Mandal, A.; Patel, B. K.

Supramolecular features of 2-(chlorophenyl)-3-(chlorobenzylidene)amino-2,3-dihydroquinazolin-4(1H)-ones: A combined experimental and computational study  
Journal of Molecular Structure, (1155): 78-89. 2018. 10.1016/j.molstruc.2017.10.085

Mandal, D.; Dhara, D.; Maiti, A.; Klemmer, L.; Huch, V.; Zimmer, M.; Rzepa, H. S.; Scheschkewitz, D.; Jana, A.

Mono- and Dicoordinate Germanium(0) as a Four-Electron Donor  
Chemistry-a European Journal, (24): 2873-2878. 2018. 10.1002/chem.201800071

Mandal, S.; Vedarajan, R.; Matsumi, N.; Ramanujam, K.

Computational Investigation of the Influence of pi-Bridge Conjugation Order of Thiophene and Thiazole Units in Triphenylamine Based Dyes in Dye-Sensitized Solar Cells  
Chemistryselect, (3): 3582-3590. 2018. 10.1002/slct.201702882

Maniei, Z.; Shakerzadeh, E.; Mahdavifar, Z.

Theoretical approach into potential possibility of efficient NO<sub>2</sub> detection via B-40 and Li@B-40 fullerenes  
Chemical Physics Letters, (691): 360-365. 2018. 10.1016/j.cplett.2017.11.045

Manna, R. N.; Grzybkowska, A.; Gelman, F.; Dybala-Defratyka, A.

Carbon-bromine bond cleavage - A perspective from bromine and carbon kinetic isotope effects on model debromination reactions  
Chemosphere, (193): 17-23. 2018. 10.1016/j.chemosphere.2017.10.153

Mansoor, E.; Head-Gordon, M.; Bell, A. T.

Computational Modeling of the Nature and Role of Ga Species for Light Alkane Dehydrogenation Catalyzed by Ga/H-MFI  
ACS Catalysis, (8): 6146-6162. 2018. 10.1021/acscatal.7b04295

Mansour, A. M.

Effect of metal complex formation on the antibacterial activity of nitazoxanide: Spectroscopic and density functional theory calculations  
Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4023

Mansour, A. M.

Structural studies and biological activity evaluation of Pd(II), Pt(II) and Ru(II) complexes containing N-phenyl, N'-(3-triazolyl)thiourea

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.3928

Manthri, S. A.; Muhamed, R. R.; Rajesh, R.; Sathyanarayananamoorthi, V.

Spectroscopic and quantum mechanical investigations of (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-phenylprop-2-enamide using density functional theory method

Indian Journal of Pure & Applied Physics, (56): 34-47. 2018.

Manzetti, S.

Quantum chemical calculations of the active site of the solute-binding protein PsaA from Streptococcus pneumoniae explain electronic selectivity of metal binding

Structural Chemistry, (29): 393-401. 2018. 10.1007/s11224-017-1036-6

Mao, Y. Z.; Ge, Q. H.; Horn, P. R.; Head-Gordon, M.

On the Computational Characterization of Charge-Transfer Effects in Noncovalently Bound Molecular Complexes

Journal of Chemical Theory and Computation, (14): 2401-2417. 2018. 10.1021/acs.jctc.7b01256

Mao, Y. Z.; Head-Gordon, M.; Shao, Y. H.

Unraveling substituent effects on frontier orbitals of conjugated molecules using an absolutely localized molecular orbital based analysis

Chemical Science, (9): 8598-8607. 2018. 10.1039/c8sc02990c

Marino, T.; Galano, A.; Mazzone, G.; Russo, N.; Alvarez-Idaboy, J. R.

Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently

Chemistry-a European Journal, (24): 8686-8691. 2018. 10.1002/chem.201800913

Mark-Lee, W. F.; Chong, Y. Y.; Kassim, M. B.

Supramolecular structures of rhenium(I) complexes mediated by ligand planarity via the interplay of substituents

Acta Crystallographica Section C-Structural Chemistry, (74): 997-+. 2018.

10.1107/s2053229618010586

Marques, I.; Costa, P. M. R.; Miranda, M. Q.; Busschaert, N.; Howe, E. N. W.; Clarke, H. J.; Haynes, C. J. E.; Kirby, I. L.; Rodilla, A. M.; Perez-Tomas, R.; Gale, P. A.; Felix, V.

Full elucidation of the transmembrane anion transport mechanism of squaramides using in silico investigations

Physical Chemistry Chemical Physics, (20): 20796-20811. 2018. 10.1039/c8cp02576b

Marquez, M. J.; Romani, D.; Diaz, S. B.; Brandan, S. A.

Structural and vibrational characterization of anhydrous and dihydrated species of trehalose based on the FTIR and FT-Raman spectra and DFT calculations

Journal of King Saud University Science, (30): 229-249. 2018. 10.1016/j.jksus.2017.01.009

Martinez-Haya, B.; Aviles-Moreno, J. R.; Gamez, F.; Berden, G.; Oomens, J.  
Preferential host-guest coordination of nonactin with ammonium and hydroxylammonium  
Journal of Chemical Physics, (149) 2018. 10.1063/1.5049956

Martins, F. A.; Freitas, M. P.  
Revisiting the Case of an Intramolecular Hydrogen Bond Network Forming Four- and Five-Membered Rings in D-Glucose  
ACS Omega, (3): 10250-10254. 2018. 10.1021/acsomega.8b01455

Mary, A.; Gupta, R.  
Effect of counterion on the reactivity, stability, aromaticity and charge distribution in mono- and polyphosphacyclopentadienide ions - A theoretical investigation  
Computational and Theoretical Chemistry, (1139): 27-37. 2018. 10.1016/j.comptc.2018.07.001

Mary, S. Y.; Al-Abdullah, E. S.; Aljohar, H. I.; Narayana, B.; Nayak, P. S.; Sarojini, B. K.; Armakovic, S.; Armakovic, S. J.; Van Alsenoy, C.; El-Emam, A. A.  
4-(4-Acetylphenyl)amino -2-methylidene-4-oxobutanoic acid, a newly synthesized amide with hydrophilic and hydrophobic segments: Spectroscopic characterization and investigation of its reactive properties  
Journal of the Serbian Chemical Society, (83): 1-18. 2018. 10.2298/jsc170103056m

Masoome, S.; Siyamak, S.; Liudmila, F.; Evgenij, D.; Mehrnoosh, K.  
DFT Investigations (Geometry Optimization, UV/Vis, FT-IR, NMR, HOMO-LUMO, FMO, MEP, NBO, Excited States) and the Syntheses of New Pyrimidine Dyes  
Chinese Journal of Structural Chemistry, (37): 1201-1222. 2018. 10.14102/j.cnki.0254-5861.2011-1887

Masson, M. A. C.; Karpfenstein, R.; de Oliveira-Silva, D.; Teuler, J. M.; Archirel, P.; Maitre, P.; Correra, T. C.  
Evaluation of Ca<sup>2+</sup> Binding Sites in Tacrolimus by Infrared Multiple Photon Dissociation Spectroscopy  
Journal of Physical Chemistry B, (122): 9860-9868. 2018. 10.1021/acs.jpcb.8b06523

Masumoto, Y.; Miyamoto, K.; Iuchi, T.; Ochiai, M.; Hirano, K.; Saito, T.; Wang, C.; Uchiyama, M.  
Mechanistic Study on Aryl-Exchange Reaction of Diaryl-lambda(3)-iodane with Aryl Iodide  
Journal of Organic Chemistry, (83): 289-295. 2018. 10.1021/acs.joc.7b02701

Masuzaki, D.; Takehashi, Y.; Mafune, F.  
Stability and Effect of Hydration on Calcium Oxide Cluster Ions, Ca<sub>n</sub>O<sub>m</sub><sup>+</sup>, in the Gas Phase  
Bulletin of the Chemical Society of Japan, (91): 1530-1536. 2018. 10.1246/bcsj.20180149

Matczak, P.  
Tuning of non-covalent interactions involving a halogen atom that plays the role of Lewis acid and base simultaneously

Molecular Physics, (116): 338-350. 2018. 10.1080/00268976.2017.1386805

Matsubara, T.; Yamasaki, R.; Hori, T.; Morikubo, M.

B equivalent to B Triple Bond of Newly Synthesized Diboryne Can Take a Different Mechanism for the sigma Bond Activation of Polar and Nonpolar Molecules. A Quantum Mechanical Study

Bulletin of the Chemical Society of Japan, (91): 1683-1690. 2018. 10.1246/bcsj.20180190

Matsu, T.; Hayakawa, N.

pi-Electron systems containing Si=Si double bonds

Science and Technology of Advanced Materials, (19): 108-129. 2018.

10.1080/14686996.2017.1414552

Matta, C. F.

Molecules as networks: A localization-delocalization matrices approach

Computational and Theoretical Chemistry, (1124): 1-14. 2018. 10.1016/j.comptc.2017.11.018

Mattock, J. D.; Vargas, A.

Boron Centres Allow Design, Control and Systematic Tuning of Neutral Homoaromatics for Functionalization Purposes

Chemphyschem, (19): 2525-2533. 2018. 10.1002/cphc.201800453

McDowell, S. A. C.

The effect of anions on noncovalent interactions in model clusters of chalcogen-containing (CH<sub>3</sub>)<sub>2</sub>X (X = O, S, Se) molecules

Physical Chemistry Chemical Physics, (20): 18420-18428. 2018. 10.1039/c8cp03641a

Mebs, S.; Kallane, S. I.; Braun, T.

Hapticity of asymmetric rhodium-allyl compounds in the light of real-space bonding indicators Zeitschrift Fur Kristallographie-Crystalline Materials, (233): 615-626. 2018. 10.1515/zkri-2017-2141

Medina, F. E.; Neves, R. P. P.; Ramos, M. J.; Fernandes, P. A.

QM/MM Study of the Reaction Mechanism of the Dehydratase Domain from Mammalian Fatty Acid Synthase

ACS Catalysis, (8): 10267-10278. 2018. 10.1021/acscatal.8602616

Mehranfar, A.; Izadyar, M.

Theoretical evaluation of symmetrical alpha,alpha ',delta,delta '-tetramethyl cucurbit 6 uril for haloalkane 1-(3-chlorophenyl)-4-(3-chloropropyl)-piperazinium and chloroform encapsulation

Journal of Inclusion Phenomena and Macrocyclic Chemistry, (92): 103-114. 2018.

10.1007/s10847-018-0820-2

Mehranfar, A.; Izadyar, M.; Shamkhali, A. N.

A joint MD/QM study on the possibility of alkaloids detection by cucurbiturils and graphene oxide-cucurbituril composites

Journal of Molecular Liquids, (272): 963-972. 2018. 10.1016/j.molliq.2018.10.092

Mehri, M.; Chafai, N.; Ouksel, L.; Benbouguerra, K.; Hellal, A.; Chafaa, S.

Synthesis, electrochemical and classical evaluation of the antioxidant activity of three alpha-aminophosphonic acids: Experimental and theoretical investigation

Journal of Molecular Structure, (1171): 179-189. 2018. 10.1016/j.molstruc.2018.05.074

Mei, Q. Q.; Liu, H. Z.; Yang, Y. D.; Liu, H. Y.; Li, S. P.; Zhang, P.; Han, B. X.

Base-Free Aerobic Oxidation of Alcohols over Copper-Based Complex under Ambient Condition  
ACS Sustainable Chemistry & Engineering, (6): 2362-2369. 2018.  
10.1021/acssuschemeng.7b03820

Mei, Q. Q.; Yang, Y. D.; Liu, H. Y.; Li, S. P.; Liu, H. Z.; Han, B. X.

A new route to synthesize aryl acetates from carbonylation of aryl methyl ethers  
Science Advances, (4) 2018. 10.1126/sciadv.aaq0266

Mejia, L.; Ferraro, F.; Osorio, E.; Hadad, C. Z.

Activation and diffusion of ammonia borane hydrogen on gold tetramers  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25567

Mejia-Olvera, R.; Reveles, J. U.; Pacheco-Ortin, S. M.; Santoyo-Salazar, J.

Molecular dynamics and electronic structure study of neutral, cationic and anionic (Fe<sub>3</sub>O<sub>4</sub>)(1-5) clusters

Chemical Physics Letters, (706): 494-500. 2018. 10.1016/j.cplett.2018.06.011

Melengate, G. S.; Stoyanov, S. R.; Quattrociocchi, D. G. S.; da Costa, L. M.; Ferreira, G. B.

Theoretical Study of the Interaction of 1,2-Dithiolene Ligands with the Mg<sup>2+</sup> and Ca<sup>2+</sup>  
Aquacations: Electronic, Geometric and Energetic Analysis

Journal of the Brazilian Chemical Society, (29): 856-872. 2018. 10.21577/0103-5053.20170210

Melichar, P.; Hnyk, D.; Fanfrlik, J.

A systematic examination of classical and multi-center bonding in heteroborane clusters  
Physical Chemistry Chemical Physics, (20): 4666-4675. 2018. 10.1039/c7cp07422k

Melis, M.; Mastinu, M.; Arca, M.; Crnjar, R.; Barbarossa, L. T.

Effect of chemical interaction between oleic acid and L-Arginine on oral perception, as a function of polymorphisms of CD36 and OBPII alpha and genetic ability to taste 6-n-propylthiouracil  
PLoS One, (13) 2018. 10.1371/journal.pone.0194953

Melo, J. P.; Rios, P. L.; Povea, P.; Morales-Verdejo, C.; Camarada, M. B.

Graphene Oxide Quantum Dots as the Support for the Synthesis of Gold Nanoparticles and Their Applications as New Catalysts for the Decomposition of Composite Solid Propellants

ACS Omega, (3): 7278-7287. 2018. 10.1021/acsomega.8b00837

Memarian, H. R.; Kalantari, M.

Electron-transfer induced oxidation of 2-oxo-1,2,3,4-tetrahydropyridines using TiO<sub>2</sub> anatase-nanoparticles: steric and electronic substitution effects

Journal of the Iranian Chemical Society, (15): 2135-2145. 2018. 10.1007/s13738-018-1407-y

Mendonca, J. G. P.; Fernandes, S. A.; Cormanich, R. A.; Freitas, M. P.

Anion effect on the conformational equilibrium of sulfamide and its N,N-diindolyl derivative: Insights on anion transportation

Journal of Physical Organic Chemistry, (31) 2018. 10.1002/poc.3850

Meng, Q. X.; Wang, F.

Mechanism for Co(dppp)-catalyzed regioselective intermolecular hydroacylation of 1,3-dienes and benzaldehydes: Insights from density functional calculations

Journal of Organometallic Chemistry, (868): 102-111. 2018. 10.1016/j.jorgancem.2018.04.042

Meng, X. T.; Yu, C.; Zhang, X. P.; Huang, L. L.; Rager, M.; Hong, J. F.; Qiu, J.; Lin, Z. Q.

Active sites-enriched carbon matrix enables efficient triiodide reduction in dye-sensitized solar cells: An understanding of the active centers

Nano Energy, (54): 138-147. 2018. 10.1016/j.nanoen.2018.09.070

Menkir, M. G.; Lee, S. L.

Density Functional Theory Study on the Mechanisms of Platinum- and Gold-Catalyzed Cycloisomerizations of Biaryl Propargyl Alcohol and Indolyl Allenol to Phenanthrene and Carbazole Chemistryselect, (3): 12093-12107. 2018. 10.1002/slct.201802239

Menon, V. V.; Mary, Y. S.; Mary, Y. S.; Panicker, C. Y.; Bielenica, A.; Armakovic, S.; Armakovic, S. J.; Van Alsenoy, C.

Combined spectroscopic, DFr, TD-DFT and MD study of newly synthesized thiourea derivative Journal of Molecular Structure, (1155): 184-195. 2018. 10.1016/j.molstruc.2017.10.093

Merzoud, L.; Saal, A.; Moussaoui, R.; Ouamerali, O.; Morell, C.; Chermette, H.

Fluorine substituent effect on the stereochemistry of catalyzed and non-catalyzed Diels-Alder reactions. The case of R-butenone with cyclopentadiene: a computational assessment of the mechanism Physical Chemistry Chemical Physics, (20): 16102-16116. 2018. 10.1039/c8cp00985f

Meshhal, M. M.; Shibli, M. F.; El-Demerdash, S. H.; El-Nahas, A. M.

A computational study on molecular structure and stability of tautomers of dipyrrole-based phenanthroline analogue

Computational and Theoretical Chemistry, (1145): 6-14. 2018. 10.1016/j.comptc.2018.10.003

Messasma, Z.; Ourari, A.; Mandadi, R.; Houchi, S.; Aggoun, D.; Kherbache, A.; Bentouhami, E.

Synthesis, spectral characterization, DFT computational studies and inhibitory activity of novel N2S2 tetridentates Schiff bases on metallo-beta-lactamases of *Acinetobacter baumannii*  
Journal of Molecular Structure, (1171): 672-681. 2018. 10.1016/j.molstruc.2018.06.044

Meza, M. P.; Sotelo, D. P.; Hernandez, M. V.; Pico, E. A.; Lopez, S. F.

Viscometric, thermodynamic and theoretical DFT studies of DL-2-aminobutyric acid in aqueous sodium nitrate solutions at different temperatures

Journal of Molecular Liquids, (271): 599-609. 2018. 10.1016/j.molliq.2018.09.012

Michalczyk, M.; Zierkiewicz, W.; Drozdzewski, P.; Nawaz, S.; Monim-ul-Mehboob, M.; Ahmad, S.

Theoretical modeling of argentophilic interactions in Ag(CN)(2)(-) (3) trimer found in a copper(II) complex of cis-1,2-diaminocyclohexane (Dach), Cu (Dach)(2)-Ag(CN)(2)-Cu(Dach)(2) Ag(CN)(2) (3)  
Chemical Physics Letters, (709): 11-15. 2018. 10.1016/j.cplett.2018.08.034

Michalczyk, M.; Zierkiewicz, W.; Scheiner, S.

Triel-Bonded Complexes between TrR3 (Tr=B, Al, Ga; R=H, F, Cl, Br, CH<sub>3</sub>) and Pyrazine  
Chemphyschem, (19): 3122-3133. 2018. 10.1002/cphc.201800774

Michenfelder, N. C.; Ernst, H. A.; Schweigert, C.; Olzmann, M.; Unterreiner, A. N.

Ultrafast stimulated emission of nitrophenolates in organic and aqueous solutions  
Physical Chemistry Chemical Physics, (20): 10713-10720. 2018. 10.1039/c7cp07774b

Mierzwa, G.; Gordon, A. J.; Berski, S.

On the nature of the boron-copper interaction. Topological study of the electron localisation function (ELF)

New Journal of Chemistry, (42): 17096-17114. 2018. 10.1039/c8nj03516d

Mikherdov, A. S.; Kinzhakov, M. A.; Novikov, A. S.; Boyarskiy, V. P.; Boyarskaya, I. A.; Avdontceva, M. S.; Kukushkin, V. Y.

Ligation-Enhanced pi-Hole center dot center dot center dot pi Interactions Involving Isocyanides: Effect of pi-Hole center dot center dot center dot pi Noncovalent Bonding on Conformational Stabilization of Acyclic Diaminocarbene Ligands

Inorganic Chemistry, (57): 6722-6733. 2018. 10.1021/acs.inorgchem.8b01027

Mikherdov, A. S.; Novikov, A. S.; Kinzhakov, M. A.; Boyarskiy, V. P.; Starova, G. L.; Ivanov, A. Y.; Kukushkin, V. Y.

Halides Held by Bifurcated Chalcogen-Hydrogen Bonds. Effect of mu Cl-(S,Cl-N-H) Contacts on Dimerization of Cl(carbene)Pd-II Species

Inorganic Chemistry, (57): 3420-3433. 2018. 10.1021/acs.inorgchem.8b00190

Mikherdov, A. S.; Novikov, A. S.; Kinzhakov, M. A.; Zolotarev, A. A.; Boyarskiy, V. P.

Intra-/Intermolecular Bifurcated Chalcogen Bonding in Crystal Structure of Thiazole/Thiadiazole Derived Binuclear (Diaminocarbene)Pd-II Complexes

Crystals, (8) 2018. 10.3390/crust8030112

Milani, N. N.; Ghiasi, R.; Forghaniha, A.

Theoretical investigation of vinylogous anomeric effect on 4-halo-4-H-pyran and 4-halo-4-H-thiopyran molecules

Journal of Sulfur Chemistry, (39): 665-673. 2018. 10.1080/17415993.2018.1513523

Milenkovic, D.; Avdovic, E. H.; Dimic, D.; Bajin, Z.; Ristic, B.; Vukovic, N.; Trifunovic, S. R.; Markovic, Z. S.

Reactivity of the coumarine derivative towards cartilage proteins: combined NBO, QTAIM, and molecular docking study

Monatshefte fur Chemie, (149): 159-166. 2018. 10.1007/s00706-017-2051-4

Milenkovic, D.; Dorovic, J.; Petrovic, V.; Avdovic, E.; Markovic, Z.

Hydrogen atom transfer versus proton coupled electron transfer mechanism of gallic acid with different peroxy radicals

Reaction Kinetics Mechanisms and Catalysis, (123): 215-230. 2018. 10.1007/s11144-017-1286-8

Mills, J. D.; Boatz, J. A.; Langhoff, P. W.

Quantum-mechanical definition of atoms and their mutual interactions in Born-Oppenheimer molecules

Physical Review A, (98) 2018. 10.1103/PhysRevA.98.012506

Milosevic, M. D.; Prlainovic, N. Z.; Milcic, M.; Nikolic, V.; Bozic, A.; Bigovic, M.; Marinkovic, A. D.

Solvent, structural, quantum chemical study and antioxidative activity of symmetrical 1-methyl-2,6-bis 2-(substituted phenyl)ethenyl pyridinium iodides

Journal of the Iranian Chemical Society, (15): 2483-2501. 2018. 10.1007/s13738-018-1437-5

Minh, N. D.; Cuong, C. H.; Trung, N. T.; Ngan, V. T.

Insight into chemical bonding of the transition metal-doped cluster Ge<sub>2</sub>M (M = Sc-Zn) series using NBO and NRT theory

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2326-9

Minteguiaga, M.; Dellacassa, E.; Iramain, M. A.; Catalan, C. A. N.; Brandan, S. A.

Synthesis, spectroscopic characterization and structural study of 2-isopropenyl-3-methylphenol, carquejiphenol, a carquejol derivative with potential medicinal use

Journal of Molecular Structure, (1165): 332-343. 2018. 10.1016/j.molstruc.2018.04.001

Miqueu, K.; Labat, S.; Carrizo, E. D. S.; Sotiropoulos, J. M.

Short-Lived Orthobenzene Complexes with Early Transition Metals of Group IV. First Direct Characterization and Electronic Cartography by Coupling FVT/UV-PES with Calculations

European Journal of Inorganic Chemistry: 2717-2729. 2018. 10.1002/ejic.201800458

Mir, N.; Jalilian, S.; Karimi, P.; Nejati-Yazdinejad, M.; Khammarnia, S.

1,3,4-Thiadiazol derivative functionalized-Fe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub> nanocomposites as a fluorescent probe for detection of Hg<sup>2+</sup> in water samples

RSC Advances, (8): 21745-21753. 2018. 10.1039/c8ra03448f

Miranda-Rojas, S.; Fernandez, I.; Kastner, J.; Toro-Labbe, A.; Mendizabal, F.

Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase

Chemcatchem, (10): 1052-1063. 2018. 10.1002/cctc.201701517

Mirzaei, M. S.; Taherpour, A. A.

Tautomeric preferences of the cis and trans isomers of axitinib

Chemical Physics, (507): 10-18. 2018. 10.1016/j.chemphys.2018.04.006

Mishra, R.; Jana, A.; Panday, A. K.; Choudhury, L. H.

Synthesis of fused pyrroles containing 4-hydroxycoumarins by regioselective metal-free multicomponent reactions

Organic & Biomolecular Chemistry, (16): 3289-3302. 2018. 10.1039/c8ob00161h

Misiak, P.; Dubis, A. T.; Lapinski, A.

Does the Intramolecular Hydrogen Bond Affect the Spectroscopic Properties of Bicyclic Diazole Heterocycles?

Journal of Spectroscopy, 2018. 10.1155/2018/1048157

Mitra, I.; Mukherjee, S.; Reddy, B. V. P.; Misini, B.; Das, P.; Dasgupta, S.; Linert, W.; Moi, S. C.

Synthesis, biological evaluation, substitution behaviour and DFT study of Pd(II) complexes incorporating benzimidazole derivative

New Journal of Chemistry, (42): 2574-2589. 2018. 10.1039/c7nj05173e

Mizrahi, A.; Maimon, E.; Cohen, H.; Kornweitz, H.; Zilbermann, I.; Meyerstein, D.

Mechanistic Studies on the Role of Cu-II(CO<sub>3</sub>)(n) (2-2n) as a Water Oxidation Catalyst: Carbonate as a Non-Innocent Ligand

Chemistry-a European Journal, (24): 1088-1096. 2018. 10.1002/chem.201703742

Mo, L. H.; Liu, Q. Y.; Zhang, T.; Li, Z. Y.; He, S. G.

Reactivity of Tantalum Carbide Cluster Anions TaC<sub>n</sub>- (n=1-4) with Dinitrogen

Journal of Physical Chemistry A, (122): 3489-3495. 2018. 10.1021/acs.jpca.8b01329

Modesto-Costa, L.; Borges, I.; Aquino, A. J. A.; Lischka, H.

Electronic structure theory gives insights into the higher efficiency of the PTB electron-donor polymers for organic photovoltaics in comparison with prototypical P3HT

Journal of Chemical Physics, (149) 2018. 10.1063/1.5054919

Modesto-Costa, L.; Martinez, S. T.; Pinto, A. C.; Vessecchi, R.; Borges, I.

Elucidating the mass spectrum of the retronecine alkaloid using DFT calculations

Journal of Mass Spectrometry, (53): 934-941. 2018. 10.1002/jms.4253

Mohajeri, A.; Omidvar, A.

Fe/N-x clusters embedded in graphene with tunable properties for gas separation  
Synthetic Metals, (241): 39-46. 2018. 10.1016/j.synthmet.2018.04.003

Mohammadi, M. D.; Hamzehloo, M.

The adsorption of bromomethane onto the exterior surface of aluminum nitride, boron nitride, carbon, and silicon carbide nanotubes: A PBC-DFT, NBO, and QTAIM study  
Computational and Theoretical Chemistry, (1144): 26-37. 2018. 10.1016/j.comptc.2018.10.001

Mohammadpour, F.; Dokooohaki, M. H.; Zolghadr, A. R.; Ghatee, M. H.; Moradi, M.

Confinement of aqueous mixtures of ionic liquids between amorphous TiO<sub>2</sub> slit nanopores: electrostatic field induction  
Physical Chemistry Chemical Physics, (10): 29493-29502. 2018. 10.1039/c8cp04500c

Mohbiya, D. R.; Sekar, N.

Tuning 'Stokes Shift' and ICT Character by Varying the Donor Group in Imidazo 1,5 a pyridines: A Combined Optical, DFT, TD-DFT and NLO Approach  
Chemistryselect, (3): 1635-1644. 2018. 10.1002/slct.201702579

Mohtat, B.; Siadati, S. A.; Khalilzadeh, M. A.; Zareyee, D.

The concern of emergence of multi-station reaction pathways that might make stepwise the mechanism of the 1,3-dipolar cycloadditions of azides and alkynes  
Journal of Molecular Structure, (1155): 58-64. 2018. 10.1016/j.molstruc.2017.10.034

Molcanov, K.; Mali, G.; Grdadolnik, J.; Stare, J.; Stilinovic, V.; Kojic-Prodic, B.

Iodide center dot center dot center dot pi Interactions of Perhalogenated Quinoid Rings in Co-crystals with Organic Bases

Crystal Growth & Design, (18): 5182-5193. 2018. 10.1021/acs.cgd.8b00634

Monascal, Y.; Cartaya, L.; Alvarez-Aular, A.; Maldonado, A.; Chuchani, G.

The ion pair mechanism in the thermal deamination of primary amines catalyzed by HBr in the gas phase: DFT and AIM analysis

Chemical Physics Letters, (703): 117-123. 2018. 10.1016/j.cplett.2018.05.015

Monascal, Y.; Gallardo, E.; Cartaya, L.; Maldonado, A.; Bentarcurt, Y.; Chuchani, G.

The keto-enol equilibrium and thermal conversion kinetics of 2-and 4-hydroxyacetophenone in the gas phase: a DFT study

Molecular Physics, (116): 194-203. 2018. 10.1080/00268976.2017.1374483

Mondal, B.; Bag, R.; Ghorai, S.; Bakthavachalam, K.; Jemmis, E. D.; Ghosh, S.

Synthesis, Structure, Bonding, and Reactivity of Metal Complexes Comprising Diborane(4) and Diborene(2): {Cp\*Mo(CO)(2)}(2){mu-eta(2)-eta(2)-B<sub>2</sub>H<sub>4</sub>} and {Cp\*M(CO)(2)}(2)B<sub>2</sub>H<sub>2</sub>M(CO)(4), M=Mo,W  
Angewandte Chemie-International Edition, (57): 8079-8083. 2018. 10.1002/anie.201803154

Mondal, B.; Bag, R.; Ghosh, S.

Combined Experimental and Theoretical Investigations of Group 6 Dimetallaboranes  
(Cp<sup>\*</sup>M)(2)B4H10 (M = Mo and W)  
Organometallics, (37): 2419-2428. 2018. 10.1021/acs.organomet.8b00204

Mondal, T.; De, S.; Dutta, S.; Koley, D.

Mechanistic Exploration of the Transmetalation and Reductive Elimination Events Involving Pd-IV-Abnormal NHC Complexes in Suzuki-Miyaura Coupling Reactions: A DFT Study  
Chemistry-a European Journal, (24): 6155-6168. 2018. 10.1002/chem.201800024

Mondragon-Solorzano, G.; Barroso-Flores, J.

Spectroscopical UV-Vis implications of an intramolecular eta(2)-Mg coordination in bacteriochlorophyll-alpha from the Fenna-Matthews-Olson complex  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25663

Monim-ul-Mehboob, M.; Ramzan, M.; Zierkiewicz, W.; Michalczyk, M.; Mahmood, R.; Altaf, M.; Nadeem, S.; Akhtar, M.; Ahmad, S.

Synthesis, Characterization, and DFT Investigation of a Zinc(II)-Silver(I) Bimetallic Complex, Zn(Dmen)(2){Ag(CN)(2)}(2) Zn(Dmen)(2)(H2O)(2) {Ag(CN)(2)}(2) (Dmen = N,N'-Dimethylethylenediamine)  
Russian Journal of Coordination Chemistry, (44): 198-206. 2018. 10.1134/s1070328418030041

Monim-ul-Mehboob, M.; Ruffer, T.; Lang, H.; Zierkiewicz, W.; Rauf, A.; Amin, M.; Isab, A. A.; Ajouyed, O.; Ahmad, S.

Synthesis, crystal structure and DFT calculations of a cyanido-bridged dinuclear zinc(II) complex of cis-1,2-diaminocyclohexane (Dach) containing a dinuclear cyanidozincate(II) anion, Zn-2(Dach)(4)(CN)Zn-2(CN)(7) center dot 2CH(3)OH  
Journal of Molecular Structure, (1169): 110-118. 2018. 10.1016/j.molstruc.2018.05.049

Montero-Campillo, M. M.; Alkorta, I.; Elguero, J.

Fostering the Basic Instinct of Boron in Boron-Beryllium Interactions

Journal of Physical Chemistry A, (122): 3313-3319. 2018. 10.1021/acs.jpca.8b01551

Montis, R.; Arca, M.; Aragoni, M. C.; Blake, A. J.; Castellano, C.; Demartin, F.; Isaia, F.; Lippolis, V.; Pintus, A.; Lenardao, E. J.; Perin, G.; O'Connor, A. E.; Thurow, S.

Structural diversity in the products formed by the reactions of 2-arylselanyl pyridine derivatives and dihalogens  
New Journal of Chemistry, (42): 10592-10602. 2018. 10.1039/c8nj00495a

Moo, J.; Kim, M.; Lim, J. S.; Kim, J.

Effect of phosphorus on the electronic and optical properties of naphthoxaphospholes: theoretical investigation  
Molecular Physics, (116): 1581-1588. 2018. 10.1080/00268976.2018.1435916

Moon, J.; Baek, H.; Kim, J.

Unusually high stability of B-12(BO)(12)(2-) achieved by boronyl ligand manipulation: Theoretical investigation

Chemical Physics Letters, (698): 72-76. 2018. 10.1016/j.cplett.2018.03.015

Moon, J.; Baek, H.; Lim, J. S.; Kim, J.

TDDFT and MS-CASPT2 Study of the Excited States of Para-Methoxymethylcinnamate  
Bulletin of the Korean Chemical Society, (39): 427-434. 2018. 10.1002/bkcs.11403

Mora, J. R.; Cervantes, C.; Marquez, E.

New Insight into the Chloroacetanilide Herbicide Degradation Mechanism through a Nucleophilic Attack of Hydrogen Sulfide

International Journal of Molecular Sciences, (19) 2018. 10.3390/ijms19102864

Morales-Bayuelo, A.; Sanchez-Marquez, J.; Jana, G.; Chattaraj, P. K.

Analyzing torqueselectivity in a series of unusual ring-opening reactions through bond reactivity indices and the adaptive natural density partitioning method

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25778

Moriou, C.; Da Silva, A. D.; Prado, M. J. V.; Denhez, C.; Plashkevych, O.; Chattopadhyaya, J.; Guillaume, D.; Clivio, P.

C2 '-F Stereoconfiguration As a Puckering Switch for Base Stacking at the Dinucleotide Level  
Journal of Organic Chemistry, (83): 2473-2478. 2018. 10.1021/acs.joc.7b03186

Moroz, I. B.; Larmier, K.; Liao, W. C.; Coperet, C.

Discerning gamma-Alumina Surface Sites with Nitrogen-15 Dynamic Nuclear Polarization Surface Enhanced NMR Spectroscopy of Adsorbed Pyridine

Journal of Physical Chemistry C, (122): 10871-10882. 2018. 10.1021/acs.jpcc.8b01823

Mortazavifar, A.; Raissi, H.

Theoretical Prediction of Adsorption Properties of Carmustine Drug on Various Sites of the Outer Surface of the Single-Walled Boron Nitride Nanotube and Investigation of Urea Effect on Drug Delivery by DFT and MD

Journal of Cluster Science, (29): 93-99. 2018. 10.1007/s10876-017-1309-7

Mosquera, M. A.; Ratner, M. A.; Schatz, G. C.

Locally coupled open subsystems: A formalism for affordable electronic structure calculations featuring fractional charges and size consistency

Journal of Chemical Physics, (149) 2018. 10.1063/1.5038557

Mostafavi, N.; Ebrahimi, A.

The estimation of H-bond and metal ion-ligand interaction energies in the G-Quadruplex center dot center dot center dot Mn+ complexes

Journal of Molecular Structure, (1161): 246-253. 2018. 10.1016/j.molstruc.2018.02.023

Mostafavi, N.; Ebrahimi, A.

The role of chlorine substituents in lichexanthones properties: the ionic and halogen bond interactions

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2294-0

Mousazadeh, H.; Safa, K. D.; Ghadari, R.

Synthesis, spectroscopic characterization, and DFT studies of 1,2,3-triazole-based organosilicon compounds

Journal of Molecular Structure, (1167): 200-208. 2018. 10.1016/j.molstruc.2018.03.072

Mu, W. H.; Cheng, R. J.; Fang, D. C.; Chass, G. A.

The pivotal role of electronics in preferred alkene over alkyne Ni-carbonyne insertions and absolute regioselectivities

Dalton Transactions, (47): 6494-6498. 2018. 10.1039/c8dt01154k

Mu, W. H.; Ma, Y.; Fang, D. C.; Wang, R.; Zhang, H. N.

Computational Insights into the Diels-Alder-alike Reactions of 1-Iodo-2-Lithio-o-Carborane with Fulvenes

Acta Chimica Sinica, (76): 55-61. 2018. 10.6023/a17080357

Mu, X. J.; Cai, K. S.; Wei, W. J.; Li, Y.; Wang, Z.; Wang, J. G.

Dependence of UV-Visible Absorption Characteristics on the Migration Distance and the Hyperconjugation Effect of a Methine Chain

Journal of Physical Chemistry C, (122): 7831-7837. 2018. 10.1021/acs.jpcc.7b12596

Mukherjee, D.; Hollerhage, T.; Leich, V.; Spaniol, T. P.; Englert, U.; Maron, L.; Okuda, J.

The Nature of the Heavy Alkaline Earth Metal-Hydrogen Bond: Synthesis, Structure, and Reactivity of a Cationic Strontium Hydride Cluster

Journal of the American Chemical Society, (140): 3403-3411. 2018. 10.1021/jacs.7b13796

Mukhopadhyay, B. P.

Recognition dynamics of trinuclear copper cluster and associated histidine residues through conserved or semi-conserved water molecules in human Ceruloplasmin: The involvement of aspartic and glutamic acid gates

Journal of Biomolecular Structure & Dynamics, (36): 3829-3842. 2018.

10.1080/07391102.2017.1401003

Mukhopadhyay, D. P.; Biswas, S.; Chattopadhyay, A.; Chakraborty, T.

Conformational Preference Determined by C-H center dot center dot center dot center dot pi Interaction of an O-H center dot center dot center dot O Hydrogen-Bonded Binary Complex of p-Fluorophenol with 2,5-Dihydrofuran: A Laser-Induced Fluorescence Spectroscopy Study

Journal of Physical Chemistry A, (122): 3787-3797. 2018. 10.1021/acs.jpca.8b01384

Muldoon, J. A.; Varga, B. R.; Deegan, M. M.; Chapp, T. W.; Eordogh, A. M.; Hughes, R. P.; Glueck, D. S.; Moore, C. E.; Rheingold, A. L.

Inversion of Configuration at the Phosphorus Nucleophile in the Diastereoselective and Enantioselective Synthesis of P-Stereogenic syn-Phosphiranes from Chiral Epoxides

Angewandte Chemie-International Edition, (57): 5047-5051. 2018. 10.1002/anie.201801427

Mulks, F. F.; Antoni, P. W.; Rominger, F.; Hashmi, A. S. K.

Cyclopropenylgold(I) Complexes as Aurated Carbenoids or Quasi-Carbenes

Advanced Synthesis & Catalysis, (360): 1810-1821. 2018. 10.1002/adsc.201701526

Mulks, F. F.; Faraji, S.; Rominger, F.; Dreuw, A.; Hashmi, A. S. K.

Highly Strained Organogold Complexes and Their Gold- or Rhodium-Catalyzed Isomerizations

Chemistry-a European Journal, (24): 71-76. 2018. 10.1002/chem.201704652

Mundlapati, V. R.; Sahoo, D. K.; Bhaumik, S.; Jena, S.; Chandrakar, A.; Biswal, H. S.

Noncovalent Carbon-Bonding Interactions in Proteins

Angewandte Chemie-International Edition, (57): 16496-16500. 2018. 10.1002/anie.201811171

Muniyandi, S.; Sundaram, R.; Kar, T.

Aluminum doping makes boron nitride nanotubes (BNNTs) an attractive adsorbent of hydrazine (N<sub>2</sub>H<sub>4</sub>)

Structural Chemistry, (29): 375-382. 2018. 10.1007/s11224-017-1034-8

Munoz-Castro, A.; Saillard, J. Y.

Au-12(SR)(6) (2-), As Smaller 8-Electron Gold Nanocluster Retaining an SP<sub>3</sub>-Core. Evaluation of Bonding and Optical Properties from Relativistic DFT Calculations

Chemphyschem, (19): 1846-1851. 2018. 10.1002/cphc.201800088

Munoz-Rugeles, L.; Galano, A.; Alvarez-Idaboy, J. R.

The other side of the superoxide radical anion: its ability to chemically repair DNA oxidized sites  
Chemical Communications, (54): 13710-13713. 2018. 10.1039/c8cc07834c

Munz, D.

How to tame a palladium terminal oxo

Chemical Science, (9): 1155-1167. 2018. 10.1039/c7sc05034h

Murthy, P. K.; Krishnaswamy, G.; Armakovic, S.; Armakovic, S. J.; Suchetan, P. A.; Desai, N. R.; Suneetha, V.; SreenivasaRao, R.; Bhargavi, G.; Kumar, D. B. A.

Structural and spectroscopic characterization, reactivity study and charge transfer analysis of the newly synthesized 2-(6-hydroxy-1-benzofuran-3-yl) acetic acid

Journal of Molecular Structure, (1162): 81-95. 2018. 10.1016/j.molstruc.2018.02.081

Murthy, P. K.; Suneetha, V.; Armakovic, S.; Armakovic, S. J.; Suchetan, P. A.; Giri, L.; Rao, R. S.

Synthesis, characterization and computational study of the newly synthetized sulfonamide molecule

Journal of Molecular Structure, (1153): 212-229. 2018. 10.1016/j.molstruc.2017.10.028

Muthukumar, M.; Bhuvaneswari, T.; Venkatesh, G.; Kamal, C.; Vennila, P.; Armakovic, S.; Armakovic, S. J.; Mary, Y. S.; Panicker, C. Y.

Synthesis, characterization and computational studies of semicarbazide derivative  
Journal of Molecular Liquids, (272): 481-495. 2018. 10.1016/j.molliq.2018.09.123

Muthuraja, P.; Shanmugavadi, T.; Beaula, T. J.; Jothy, V. B.; Dhandapani, M.

Influence of intramolecular hydrogen bonding interaction on the molecular properties of N-p-tolyl-5-oxo pyrrolidine-3-carboxylic acid: A theoretical and experimental study

Chemical Physics Letters, (691): 114-121. 2018. 10.1016/j.cplett.2017.11.003

Muya, J. T.; Chung, H.; Lee, S. U.

Theoretical investigation on the ground state properties of the hexaamminecobalt(III) and nitro-nitrito linkage isomerism in pentaamminecobalt(III) in vacuo  
RSC Advances, (8): 3328-3342. 2018. 10.1039/c7ra11603a

Muz, I.; Kurban, M.

Ab initio study of structural and electronic properties of  $\text{Si}_{n}\text{C}_{5-n}\text{H}_8$  ( $n=0-5$ ) series: Probing the 2D to 3D structural transition  
Inorganica Chimica Acta, (477): 318-325. 2018. 10.1016/j.ica.2018.03.008

Nabavi, S. H.; Khodabandeh, M. H.; Golbabaei, M.; Moshaii, A.; Davari, M. D.

Excited states study reveals the twisted geometry induced large stokes shift in DCM fluorescent dye

Journal of Photochemistry and Photobiology a-Chemistry, (354): 127-138. 2018.  
10.1016/j.jphotochem.2017.05.017

Nadeem, M.; Bhatti, M. H.; Zierkiewicz, W.; Bienko, D.; Yunus, U.; Shah, S. R.; Mehmood, M.; Florke, U.

Synthesis, crystal structure and NLO study of two new versatile Ca (II) complexes  
Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4564

Nagarajan, V.; Chandramouli, R.

Investigation of NH<sub>3</sub> adsorption behavior on graphdiyne nanosheet and nanotubes: A first-principles study

Journal of Molecular Liquids, (249): 24-32. 2018. 10.1016/j.molliq.2017.11.007

Nagarajan, V.; Chandramouli, R.

Investigation on adsorption properties of CO and NO gas molecules on aluminene nanosheet: A density functional application

Materials Science and Engineering B-Advanced Functional Solid-State Materials, (229): 193-200.  
2018. 10.1016/j.mseb.2017.12.015

- Nageswari, G.; George, G.; Ramalingam, S.; Govindarajan, M.  
Electronic and vibrational spectroscopic (FT-IR and FT-Raman) investigation using ab initio (HF) and DFT (B3LYP and B3PW91) and HOMO/LUMO/MEP analysis on the structure of L-serine methyl ester hydrogen chloride  
*Journal of Molecular Structure*, (1166): 422-441. 2018. 10.1016/j.molstruc.2018.04.014
- Naili, N.; Zouchoune, B.  
Structural diversity of homobinuclear transition metal complexes of the phenazine ligand: theoretical investigation  
*Structural Chemistry*, (29): 725-739. 2018. 10.1007/s11224-017-1064-2
- Nair, L. C. S.; Balachandran, S.; Dhas, D. A.; Joe, I. H.  
In-silico analysis of substituent effect on the static first order hyperpolarizability of electron donating mono substituted Chalcone derivatives  
*Journal of Molecular Modeling*, (24) 2018. 10.1007/s00894-018-3650-7
- Najafian, A.; Cundari, T. R.  
Computational study of acetylene hydration by bio-inspired group six catalyst models  
*Polyhedron*, (154): 114-122. 2018. 10.1016/j.poly.2018.07.044
- Nakajima, T.; Kamiryo, Y.; Hachiken, K.; Nakamae, K.; Ura, Y.; Tanase, T.  
Tri- and Tetranuclear Copper Hydride Complexes Supported by Tetradentate Phosphine Ligands  
*Inorganic Chemistry*, (57): 11005-11018. 2018. 10.1021/acs.inorgchem.8b01628
- Nakamura, T.; Kudo, T.  
Theoretical molecular design of hexasilabenzene analogues aiming for the thermodynamic and kinetic stabilization  
*Computational and Theoretical Chemistry*, (1123): 61-72. 2018. 10.1016/j.comptc.2017.11.008
- Nakazawa, T.  
Density functional theory study on the geometric and electronic structures of Fe<sub>2</sub>O<sub>2</sub> and the reaction of Fe-2 + O-2  
*Computational Materials Science*, (146): 334-345. 2018. 10.1016/j.commatsci.2017.11.027
- Nakhaei, E.; Nowroozi, A.; Ravari, F.  
The hydrogen-bonded complexes of the 5-fluorouracil with the DNA purine bases: a comprehensive quantum chemical study  
*Structural Chemistry*, (29): 69-80. 2018. 10.1007/s11224-017-1001-4
- Nardini, V.; Dias, L. G.; Palaretti, V.; da Silva, G. V. J.  
Citronellal assumes a folded conformation in solution due to dispersion interactions: A joint NMR-DFT analysis  
*Journal of Molecular Structure*, (1157): 401-407. 2018. 10.1016/j.molstruc.2017.12.083

- Naseer, M. M.; Bauza, A.; Alnasr, H.; Jurkschat, K.; Frontera, A.  
Lone pair-pi vs. sigma-hole-pi interactions in bromine head-containing oxacalix 2 arene 2 triazines  
*Crystengcomm*, (20): 3251-3257. 2018. 10.1039/c8ce00666k
- Nataraj, A.; Beena, T.; Sudha, L.; Narayana, B.; Balachandran, V.  
Spectroscopic characterization and quantum chemical investigation of molecular structure and vibrational spectra of phthalazine-1(2H)-one  
*Indian Journal of Pure & Applied Physics*, (56): 802-813. 2018.
- Nath, M. J.; Roy, S. D. D.; Joe, I. H.  
Synthesis and electronic structure studies of a novel nonlinear optical crystal L-leucinium squareate monohydrate: A spectroscopic view  
*Journal of Physics and Chemistry of Solids*, (122): 143-153. 2018. 10.1016/j.jpcs.2018.06.025
- Nath, S. R.; Joshi, K. A.  
Mechanistic investigation in the 1,4 and 1,2 Wittig rearrangement reactions: a DFT study  
*Physical Chemistry Chemical Physics*, (20): 21457-21473. 2018. 10.1039/c8cp01045e
- Navarro-Ibarra, D. C.; Aguilera-Granja, J. F.; Guirado-Lopez, R. A.  
Vibrational properties of small rhodium clusters: role of magnetism, charge state, and isomerization effects  
*European Physical Journal D*, (72) 2018. 10.1140/epjd/e2018-80750-6
- Nebgen, B.; Lubbers, N.; Smith, J. S.; Sifain, A. E.; Lokhov, A.; Isayev, O.; Roitberg, A. E.; Barros, K.; Tretiak, S.  
Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks  
*Journal of Chemical Theory and Computation*, (14): 4687-4698. 2018. 10.1021/acs.jctc.8b00524
- Nemati-Kande, E.; Abbasi, M.; Mohammadi, M. D.  
DFT, QTAIM and NBO Investigation of the Interaction of Rare Gases with Pristine and Decorated Boron Nitride Nanotube  
*Chemistryselect*, (3): 9833-9840. 2018. 10.1002/slct.201802003
- Nemes, C. T.; Laconsay, C. J.; Galbraith, J. M.  
Hydrogen bonding from a valence bond theory perspective: the role of covalency  
*Physical Chemistry Chemical Physics*, (20): 20963-20969. 2018. 10.1039/c8cp03920h
- Nemytova, N. A.; Shchegol'kov, E. V.; Burgart, Y. V.; Slepukhin, P. A.; Borisevich, S. S.; Khursan, S. L.; Saloutin, V. I.  
Regiocontrolled N-, O- and C-methylation of 1-phenyl-3-polyfluoroalkyl-1H-pyrazol-5-ols  
*Journal of Fluorine Chemistry*, (206): 72-81. 2018. 10.1016/j.jfluchem.2017.12.011

Nguyen, S. T.; Ellington, T. L.; Allen, K. E.; Gorden, J. D.; Rheingold, A. L.; Tschumper, G. S.; Hammer, N. I.; Watkins, D. L.

Systematic Experimental and Computational Studies of Substitution and Hybridization Effects in Solid-State Halogen Bonded Assemblies

Crystal Growth & Design, (18): 3244-3254. 2018. 10.1021/acs.cgd.8b00398

Nicolaou, M.; Papanikolaou, M. G.; Tsipis, A. C.; Kabanos, T. A.; Keramidas, A. D.; Sproules, S.; Miras, H. N.

Design and Assembly of Covalently Functionalised Polyoxofluorovanadate Molecular Hybrids  
Chemistry-a European Journal, (24): 3836-3845. 2018. 10.1002/chem.201705730

Niemann, T.; Stange, P.; Strate, A.; Ludwig, R.

Like-likes-Like: Cooperative Hydrogen Bonding Overcomes Coulomb Repulsion in Cationic Clusters with Net Charges up to Q=+6e

Chemphyschem, (19): 1691-1695. 2018. 10.1002/cphc.201800293

Nieto, P.; Muller, D.; Sheldrick, A.; Gunther, A.; Miyazaki, M.; Dopfer, O.

Effect of alkali ions on optical properties of flavins: vibronic spectra of cryogenic M(+)lumichrome ions (M = Li-Cs) in the gas phase

Physical Chemistry Chemical Physics, (20): 22148-22158. 2018. 10.1039/c8cp03950j

Nikolaienko, T. Y.; Bulavin, L. A.

Atomic charges for conformationally rich molecules obtained through a modified principal component regression

Physical Chemistry Chemical Physics, (20): 2890-2903. 2018. 10.1039/c7cp05703b

Nikolaienko, T. Y.; Kryachko, E. S.; Dolgonos, G. A.

On the Existence of He-He Bond in the Endohedral Fullerene He-2@C-60

Journal of Computational Chemistry, (39): 1090-1102. 2018. 10.1002/jcc.25061

Ning, Y. T.; Kawahata, M.; Yamaguchi, K.; Otani, Y.; Ohwada, T.

Synthesis, structure and N-N bonding character of 1,1-disubstituted indazolium hexafluorophosphate

Chemical Communications, (54): 1881-1884. 2018. 10.1039/c8cc00183a

Ning, Y. T.; Otani, Y.; Ohwada, T.

Contrasting C- and O-Atom Reactivities of Neutral Ketone and Enolate Forms of 3-Sulfonyloxyimino-2-methyl-1-phenyl-1-butanones

Journal of Organic Chemistry, (83): 203-219. 2018. 10.1021/acs.joc.7b02573

Nishi, N.; Sueoka, K.; Iijima, K.; Sawa, R.; Takahashi, D.; Toshima, K.

Stereospecific beta-L-Rhamnopyranosylation through an S(N)i-Type Mechanism by Using Organoboron Reagents

Angewandte Chemie-International Edition, (57): 13858-13862. 2018. 10.1002/anie.201808045

Nolle, R.; Achazi, A. J.; Kaghazchi, P.; Winter, M.; Placke, T.  
Pentafluorophenyl Isocyanate as an Effective Electrolyte Additive for Improved Performance of Silicon-Based Lithium-Ion Full Cells  
ACS Applied Materials & Interfaces, (10): 28187-28198. 2018. 10.1021/acsami.8b07683

Noormohammadbeigi, M.; Shamlouei, H. R.  
The Effect of Superalkali M<sub>3</sub>O (M = Li, Na and K) on Structure, Electrical and Nonlinear Optical Properties of C-20 Fullerene Nanocluster  
Journal of Inorganic and Organometallic Polymers and Materials, (28): 110-120. 2018.  
10.1007/s10904-017-0730-6

Nori-Shargh, D.; Weinhold, F.  
Natural Bond Orbital Theory of Pseudo-Jahn-Teller Effects  
Journal of Physical Chemistry A, (122): 4490-4498. 2018. 10.1021/acs.jpca.7b12810

Norozi-Shad, N.; Gholizadeh, M.; Izadyar, M.  
Direct C2-arylation of quinoline N-oxides by boronic esters; a molecular approach on the efficient metal-free method in C-C cross-coupling reactions  
Research on Chemical Intermediates, (44): 657-673. 2018. 10.1007/s11164-017-3126-x

Noss, M. E.; Hylden, A. T.; Carroll, P. J.; Berry, D. H.  
Electrochemistry of Ruthenium Bis(imino)pyridine Compounds: Evidence for an ECE Mechanism and Isolation of Mono and Dicationic Complexes  
Inorganic Chemistry, (57): 435-445. 2018. 10.1021/acs.inorgchem.7b02677

Novikov, A. S.; Ivanov, D. M.; Bikbaeva, Z. M.; Bokach, N. A.; Kukushkin, V. Y.  
Noncovalent Interactions Involving Iodofluorobenzenes: The Interplay of Halogen Bonding and Weak Ip(O)center dot center dot pi-Hole(arene) Interactions  
Crystal Growth & Design, (18): 7641-7654. 2018. 10.1021/acs.cgd.8b01457

Nowroozi, A.; Ebrahimi, A.; Rad, O. R.  
Mutual effects of the cation-pi, anion-pi and intramolecular hydrogen bond in the various complexes of 1,3,5-triamino-2,4,6-trinitrobenzene with some cations (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>) and anions (F, Cl, Br)  
Structural Chemistry, (29): 129-137. 2018. 10.1007/s11224-017-1010-3

Ntombela, T.; Fakhar, Z.; Ibeji, C. U.; Govender, T.; Maguire, G. E. M.; Lamichhane, G.; Kruger, H. G.; Honarpourvar, B.  
Molecular insight on the non-covalent interactions between carbapenems and I,d-transpeptidase 2 from Mycobacterium tuberculosis: ONIOM study  
Journal of Computer-Aided Molecular Design, (32): 687-701. 2018. 10.1007/s10822-018-0121-2

Nunes, C. M.; Pinto, S. M. V.; Reva, I.; Rosado, M. T. S.; Fausto, R.

Photochemistry of matrix-isolated 3-chloro-1,2-benzisoxazole: Generation and characterization of 2-cyanophenoxy radical and other reactive intermediates

Journal of Molecular Structure, (1172): 33-41. 2018. 10.1016/j.molstruc.2017.11.009

Obenchain, D. A.; Spada, L.; Alessandrini, S.; Rampino, S.; Herbers, S.; Tasinato, N.; Mendolicchio, M.; Kraus, P.; Gauss, J.; Puzzarini, C.; Grabow, J. U.; Barone, V.

Unveiling the Sulfur-Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond

Angewandte Chemie-International Edition, (57): 15822-15826. 2018. 10.1002/anie.201810637

Ohashi, S.; Iguchi, D.; Heyl, T. R.; Froimowicz, P.; Ishida, H.

Quantitative studies on the p-substituent effect of the phenolic component on the polymerization of benzoxazines

Polymer Chemistry, (9): 4194-4204. 2018. 10.1039/c8py00760h

Ohlin, C. A.; Pascual-Borras, M.

Protonation and water exchange kinetics in sandwich polyoxometalates

Dalton Transactions, (47): 13602-13607. 2018. 10.1039/c8dt02342e

Oishi, M.; Kajiwara, M.

Synthesis and Structural Features of a Lithium Borate Derived from 2,2-Dipropylglycolic Acid

Bulletin of the Chemical Society of Japan, (91): 12-18. 2018. 10.1246/bcsj.20170236

Ojha, D.; Karhan, K.; Kuhne, T. D.

On the Hydrogen Bond Strength and Vibrational Spectroscopy of Liquid Water

Scientific Reports, (8) 2018. 10.1038/s41598-018-35357-9

Okiyama, Y.; Nakano, T.; Watanabe, C.; Fukuzawa, K.; Mochizuki, Y.; Tanaka, S.

Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poisson-Boltzmann Equation: Implementation and DNA Study

Journal of Physical Chemistry B, (122): 4457-4471. 2018. 10.1021/acs.jpcb.8b01172

Okur, M.; Albayrak, N.; Tamer, O.; Avci, D.; Atalay, Y.

A Theoretical Study on N<sup>1</sup>- (Z)-(4-Methylphenyl)Methylidene -4-Nitrobenzohydrazide (NMPMN)

Brazilian Journal of Physics, (48): 398-405. 2018. 10.1007/s13538-018-0573-9

Olaru, M.; Duvinage, D.; Lork, E.; Mebs, S.; Beckmann, J.

Heavy Carbene Analogues: Donor-Free Bismuthenium and Stibenium Ions

Angewandte Chemie-International Edition, (57): 10080-10084. 2018. 10.1002/anie.201803160

Olesiejuk, M.; Kudelko, A.; Gajda, K.; Dziuk, B.; Ejsmont, K.

pi-Electron delocalization in 2-benzoyl-5-phenylpyrazolidin-3-one

Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (73): 577-582. 2018.

10.1515/znb-2018-0072

Oliaey, A. R.; Shiroudi, A.; Zahedi, E.; Deleuze, M. S.

Theoretical study on the elimination kinetics in the gas phase of allyl methyl compounds

Monatshefte fur Chemie, (149): 1389-1400. 2018. 10.1007/s00706-018-2184-0

Oliaey, A. R.; Shiroudi, A.; Zahedi, E.; Deleuze, M. S.

Theoretical study on the mechanisms and kinetics of the beta-elimination of 2,2-

dihaloethyltrihalosilanes (X = F, Cl, Br) compounds: a DFT study along with a natural bond orbital analysis

Reaction Kinetics Mechanisms and Catalysis, (124): 27-44. 2018. 10.1007/s11144-017-1332-6

Oliva-Enrich, J. M.; Humbel, S.; Santaballa, J. A.; Alkorta, I.; Notario, R.; Davalos, J. Z.; Canle-L, M.; Bernhardt, E.; Holub, J.; Hnyk, D.

Predicted Gas-Phase and Liquid-Phase Acidities of Carborane Carboxylic and Dicarboxylic Acids

Chemistryselect, (3): 4344-4353. 2018. 10.1002/slct.201800683

Olsson, S.; Dahlstrand, C.; Gogoll, A.

Design of oxophilic metalloporphyrins: an experimental and DFT study of methanol binding

Dalton Transactions, (47): 11572-11585. 2018. 10.1039/c8dt02432d

Omidvar, A.

Catalytic role of transition metals supported on niobium oxide in O<sub>2</sub> activation

Applied Surface Science, (434): 1239-1247. 2018. 10.1016/j.apsusc.2017.11.239

Omidvar, A.

Charge-controlled switchable CO adsorption on FeN<sub>4</sub> cluster embedded in graphene

Surface Science, (668): 117-124. 2018. 10.1016/j.susc.2017.10.032

Omidvar, A.

Design of a Novel Series of Donor-Acceptor Frameworks via Superalkali-Superhalogen

Assemblage to Improve the Nonlinear Optical Responses

Inorganic Chemistry, (57): 9335-9347. 2018. 10.1021/acs.inorgchem.8b01322

Omidvar, B. A.; Tayyari, S. F.; Vakili, M.; Nekoei, A. R.

Vibrational spectra, normal coordinate analysis, and hydrogen bond investigation of pyridinium perchlorate

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (191): 558-565. 2018.

10.1016/j.saa.2017.10.067

Orenha, R. P.; Tfouni, E.; Galembeck, S. E.

How does the total charge and isomerism influence the Ru-NO ammine complexes?

Physical Chemistry Chemical Physics, (20): 13348-13356. 2018. 10.1039/c8cp00865e

Orenha, R. P.; Vessecchi, R.; Galembeck, S. E.

The influence of the negative hyperconjugation is relevant for the analysis of the pi-pi\* conjugation with the mono-substitution and di-substitution of H2C= by O= and/or HN= in trans-but-1,3-diene?

Structural Chemistry, (29): 847-857. 2018. 10.1007/s11224-017-1070-4

Orief, M. I.; Abdel-Rhman, M. H.

Molecular modeling, spectroscopic and structural studies on newly synthesized ligand N-benzoyl-2-isonicotinoylhydrazine-1-carboxamide

Journal of Molecular Structure, (1173): 332-340. 2018. 10.1016/j.molstruc.2018.05.107

Orms, N.; Rehn, D. R.; Dreuw, A.; Krylov, A. I.

Characterizing Bonding Patterns in Diradicals and Triradicals by Density-Based Wave Function Analysis: A Uniform Approach

Journal of Chemical Theory and Computation, (14): 638-648. 2018. 10.1021/acs.jctc.7b01012

Orozco-Valencia, U.; Gazquez, J. L.; Vela, A.

Global and local charge transfer in electron donor-acceptor complexes

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3772-y

Orozco-Valencia, U.; Gazquez, J. L.; Vela, A.

Role of Reaction Conditions in the Global and Local Two Parabolas Charge Transfer Model

Journal of Physical Chemistry A, (122): 1796-1806. 2018. 10.1021/acs.jpca.7b12001

Ortolan, A. O.; Caramori, G. F.; Parreira, R. L. T.; Munoz-Castro, A.

Helicenes as Molecular Tweezers in the Formation of Cation- Complexes. Bonding and Circular Dichroism Properties from Relativistic DFT Calculations

Chemphyschem, (19): 2321-2330. 2018. 10.1002/cphc.201800470

Ortolan, A. O.; Oestrom, I.; Caramori, G. F.; Parreira, R. L. T.; Munoz-Castro, A.; Bickelhaupt, F. M.

Anion Recognition by Organometallic Calixarenes: Analysis from Relativistic DFT Calculations

Organometallics, (37): 2167-2176. 2018. 10.1021/acs.organomet.8b00292

Ortolan, A. O.; Ostrom, I.; Caramori, G. F.; Parreira, R. L. T.; da Silva, E. H.; Bickelhaupt, F. M.

Tuning Heterocalixarenes to Improve Their Anion Recognition: A Computational Approach

Journal of Physical Chemistry A, (122): 3328-3336. 2018. 10.1021/acs.jpca.8b01866

Oshita, H.; Yoshimura, T.; Mori, S.; Tani, F.; Shimazaki, Y.; Yamauchi, O.

Characterization of the one-electron oxidized Cu(II)-salen complexes with a side chain aromatic ring: the effect of the indole ring on the Cu(II)-phenoxyl radical species

Journal of Biological Inorganic Chemistry, (23): 51-59. 2018. 10.1007/s00775-017-1508-6

Osman, H. H.; Andres, J.; Salvado, M. A.; Recio, J. M.

Chemical Bond Formation and Rupture Processes: An Application of DFT-Chemical Pressure Approach

Journal of Physical Chemistry C, (122): 21216-21225. 2018. 10.1021/acs.jpcc.8b06947

Osman, H. H.; Salvado, M. A.; Pertierra, P.; Engelkemier, J.; Fredrickson, D. C.; Recio, J. M.

Chemical Pressure Maps of Molecules and Materials: Merging the Visual and Physical in Bonding Analysis

Journal of Chemical Theory and Computation, (14): 104-114. 2018. 10.1021/acs.jctc.7b00943

Ostrom, I.; Ortolan, A. O.; Schneider, F. S. S.; Caramori, G. F.; Parreira, R. L. T.

Quest for Insight into Ultrashort C-H center dot center dot center dot pi Proximities in Molecular "Iron Maidens"

Journal of Organic Chemistry, (83): 5114-5122. 2018. 10.1021/acs.joc.8b00461

Otyotov, A. A.; Merlyan, A. P.; Veretennikov, V. V.; Pogonin, A. E.; Ivanov, E. N.; Filippova, Y. E.; Zhabanov, Y. A.; Islyaikin, M. K.

Intramolecular Hydrogen Bonding and Electronic Structure of Thiadiazole Annulated Hemihexaphyrazine

Macroheterocycles, (11): 67-72. 2018. 10.6060/mhc1801750

Otten, B. M.; Melancon, K. M.; Omary, M. A.

All That Glitters Is Not Gold: A Computational Study of Covalent vs Metallophilic Bonding in Bimetallic Complexes of d(10) Metal CentersA Tribute to Al Cotton on the Tenth Anniversary of His Passing

Comments on Inorganic Chemistry, (38): 1-35. 2018. 10.1080/02603594.2018.1467315

Ou, T.; Feng, Y.; Tian, W. J.; Zhao, L. J.; Kong, X. Y.; Xu, H. G.; Zheng, W. J.; Zhai, H. J.

A photoelectron spectroscopy and quantum chemical study on ternary Al-B-O clusters:  
Al(n)BO(2)(-)and AlnBO2 (n=2, 3)

Physical Chemistry Chemical Physics, (20): 5200-5209. 2018. 10.1039/c7cp08512e

Ouilia, S.; Beghidja, C.; Beghidja, A.; Belkhiri, L.; Rabu, P.

Synthesis, crystal structure, magnetic properties and DFT calculations of new dihydroxo-bridged binuclear chromium(III) based on monodentate mixed ligand

Inorganica Chimica Acta, (476): 54-60. 2018. 10.1016/j.ica.2018.02.024

Padash, R.; Jafari, A. H.; Jamalizadeh, E.

Experimental and theoretical study of aluminium corrosion in NaOH, NaCl and HCl solutions  
Anti-Corrosion Methods and Materials, (65): 350-360. 2018. 10.1108/acmm-04-2017-1785

Paghandeh, H.; Saeidian, H.

Expedient and click synthesis, spectroscopic characterizations and DFT calculations of novel 1,5-bis(N-substituted 1,2,3-triazole) benzodiazepinedione scaffolds

Journal of Molecular Structure, (1157): 560-566. 2018. 10.1016/j.molstruc.2017.12.035

Pakiari, A. H.; Salarhaji, M.

Introducing nano-particle-type properties of Ti-n (n=2-6) clusters  
Journal of Molecular Graphics & Modelling, (85): 294-303. 2018. 10.1016/j.jmgm.2018.09.007

Pal, R.; Mebs, S.; Shi, M. W.; Jayatilaka, D.; Krzeszczakowska, J. M.; Malaspina, L. A.; Wiecko, M.; Luger, P.; Hesse, M.; Chen, Y. S.; Beckmann, J.; Grabowsky, S.

Linear MgCp<sub>2</sub>\* vs Bent CaCp<sub>2</sub>\*: London Dispersion, Ligand-Induced Charge Localizations, and Pseudo-Pregostic C-H center dot center dot center dot Ca Interactions

Inorganic Chemistry, (57): 4906-4920. 2018. 10.1021/acs.inorgchem.7b03079

Pal, R.; Reddy, M. B. M.; Dinesh, B.; Venkatesha, M. A.; Grabowsky, S.; Jelsch, C.; Row, T. N. G.  
&ITSyn &ITVs &ITAnti &ITCarboxylic Acids in Hybrid Peptides: Experimental and Theoretical Charge Density and Chemical Bonding Analysis

Journal of Physical Chemistry A, (122): 3665-3679. 2018. 10.1021/acs.jpca.7b10939

Palafox, M. A.; Kattan, D.; Afseth, N. K.

FT-IR spectra of the anti-HIV nucleoside analogue d4T (Stavudine). Solid state simulation by DFT methods and scaling by different procedures

Journal of Molecular Structure, (1157): 587-601. 2018. 10.1016/j.molstruc.2017.12.079

Palafox, M. A.; Rastogi, V. K.; Singh, S. P.

FT-IR and FT-Raman spectra of 5-chlorocytosine: Solid state simulation and tautomerism. Effect of the chlorine substitution in the Watson-Crick base pair 5-chlorodeoxycytidine-deoxyguanosine

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (188): 418-435. 2018. 10.1016/j.saa.2017.07.018

Palinkas, N.; Kollar, L.; Kegl, T.

Palladium-Catalyzed Synthesis of Amidines via tert-Butyl isocyanide Insertion

ACS Omega, (3): 16118-16126. 2018. 10.1021/acsomega.8b02010

Pan, J.; Cao, D. L.; Ren, F. D.; Wang, J. L.; Yang, L.

Theoretical investigation into the cooperativity effect between the intermolecular . and H-bonding interactions in the curcumin.cytosine.H<sub>2</sub>O system

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3836-z

Pan, R. K.; Wang, Y.; Song, J. L.; Liu, S. G.

Two cadmium(II) complexes derived from bidentate bis(benzoimidazol-2-ylmethyl)cyclohexane ligands: synthesis, crystal structures, spectroscopic and DFT calculations

Chemical Papers, (72): 2181-2191. 2018. 10.1007/s11696-018-0475-x

Pan, S.; Cabellos, J. L.; Orozco-Ic, M.; Chattaraj, P. K.; Zhao, L. L.; Merino, G.

Planar pentacoordinate carbon in CGa<sub>5</sub><sup>+</sup> derivatives

Physical Chemistry Chemical Physics, (20): 12350-12355. 2018. 10.1039/c8cp01009a

Pan, S.; Ghara, M.; Kar, S.; Zarate, X.; Merino, G.; Chattaraj, P. K.

Noble gas encapsulated B-40 cage

Physical Chemistry Chemical Physics, (20): 1953-1963. 2018. 10.1039/c7cp07890k

Pan, S.; Jana, G.; Ravell, E.; Zarate, X.; Osorio, E.; Merino, G.; Chattaraj, P. K.

Stable NC<sub>n</sub>gNSi (Ng= Kr, Xe, Rn) Compounds with Covalently Bound C-Ng-N Unit: Possible Isomerization of NCNSi through the Release of the Noble Gas Atom

Chemistry-a European Journal, (24): 2879-2887. 2018. 10.1002/chem.201705112

Pan, S.; Kar, S.; Saha, R.; Osorio, E.; Zarate, X.; Zhao, L. L.; Merino, G.; Chattaraj, P. K.

Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound M (c) B-10(-) Clusters (M=Nb, Ta)

Chemistry-a European Journal, (24): 3590-3598. 2018. 10.1002/chem.201705790

Pan, S.; Zhao, L. L.; Dias, H. V. R.; Frenking, G.

Bonding in Binuclear Carbonyl Complexes M-2(CO)(9) (M = Fe, Ru, Os)

Inorganic Chemistry, (57): 7780-7791. 2018. 10.1021/acs.inorgchem.8b00851

Pan, Y.; Zhao, A. J.; Li, Y.; Li, W. Q.; So, Y. M.; Yan, X. M.; He, G. H.

Bis(oxazoline)-derived N-heterocyclic carbene ligated rare-earth metal complexes: synthesis, structure, and polymerization performance

Dalton Transactions, (47) 2018. 10.1039/c8dt02130a

Panchal, M.; Kongor, A.; Athar, M.; Mehta, V.; Jha, P. C.; Jain, V. K.

Sensing of Ce(III) using di-naphthoylated oxacalix 4 arene via realistic simulations and experimental studies

New Journal of Chemistry, (42): 311-317. 2018. 10.1039/c7nj02828h

Panda, S.; Kundu, K.; Basaiahgari, A.; Singh, A. P.; Senapati, S.; Gardas, R. L.

Aggregation behaviour of biocompatible choline carboxylate ionic liquids and their interactions with biomolecules through experimental and theoretical investigations

New Journal of Chemistry, (42): 7105-7118. 2018. 10.1039/c8nj00336j

Pande, S.; Jian, T.; Khetrapal, N. S.; Wang, L. S.; Zeng, X. C.

Structural Evolution of Gold-Doped Bismuth Clusters AuBin- (n=4-8)

Journal of Physical Chemistry C, (122): 6947-6954. 2018. 10.1021/acs.jpcc.8b00166

Pandey, B.; Ray, K.; Rajaraman, G.

Structure, Bonding, Reactivity and Spectral Features of Putative N<sub>IIII</sub> = O Species: A Theoretical Perspective

Zeitschrift fur Anorganische und Allgemeine Chemie, (644): 790-800. 2018.

10.1002/zaac.201800122

Panova, Y. S.; Sheyanova, A. V.; Zolotareva, N. V.; Sushev, V. V.; Arapova, A. V.; Novikov, A. S.; Baranov, E. V.; Fukin, G. K.; Kornev, A. N.

2,2'-Azobispyridine in Phosphorus Coordination Chemistry: A New Approach to 1,2,4,3-Triazaphosphole Derivatives

European Journal of Inorganic Chemistry: 4245-4254. 2018. 10.1002/ejic.201800831

Parambil, P. C.; Hoffmann, R.

Alkyl Isosteres

Journal of the American Chemical Society, (140): 12844-12852. 2018. 10.1021/jacs.8b06141

Paria, S.; Morimoto, Y.; Ohta, T.; Okabe, S.; Sugimoto, H.; Ogura, T.; Itoh, S.

Copper(I)-Dioxygen Reactivity in the Isolated Cavity of a Nanoscale Molecular Architecture

European Journal of Inorganic Chemistry: 1976-1983. 2018. 10.1002/ejic.201800029

Parida, R.; Reddy, G. N.; Ganguly, A.; Roymahapatra, G.; Chakraborty, A.; Giri, S.

On the making of aromatic organometallic superalkali complexes

Chemical Communications, (54): 3903-3906. 2018. 10.1039/c8cc01170b

Parke, S. M.; Narreto, M. A. B.; Hupf, E.; McDonald, R.; Ferguson, M. J.; Hegmann, F. A.; Rivard, E.

Understanding the Origin of Phosphorescence in Bismoles: A Synthetic and Computational Study  
Inorganic Chemistry, (57): 7536-7549. 2018. 10.1021/acs.inorgchem.8b00149

Parvin, M. H.; Azizi, E.; Arjomandi, J.; Lee, J. Y.

Highly sensitive and selective electrochemical sensor for detection of vitamin B12 using an

Au/PPy/FMNP@TD-modified electrode

Sensors and Actuators B-Chemical, (261): 335-344. 2018. 10.1016/j.snb.2018.01.168

Patel, N.; Arfeen, M.; Sood, R.; Khullar, S.; Chakraborti, A. K.; Mandal, S. K.; Bharatam, P. V.

Can Remote N-Heterocyclic Carbenes Coordinate with Main Group Elements? Synthesis,

Structure, and Quantum Chemical Analysis of N+-Centered Complexes

Chemistry-a European Journal, (24): 6418-6425. 2018. 10.1002/chem.201705999

Patel, N.; Falke, B.; Bharatam, P. V.

C → N coordination bonds in (CCC) → N+ <- (L) complexes

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2208-1

Patel, R. N.; Singh, Y.; Singh, Y. P.; Patel, A. K.; Patel, N.; Singh, R.; Butcher, R. J.; Jasinski, J. P.; Colacio, E.; Palacios, M. A.

Varying structural motifs, unusual X-band electron paramagnetic spectra, DFT studies and superoxide dismutase enzymatic activity of copper(II) complexes with N'- (E)-phenyl(pyridin-2-yl)methylidene benzohydrazide

New Journal of Chemistry, (42): 3112-3136. 2018. 10.1039/c7nj04182a

Patil, D. S.; Avhad, K. C.; Sekar, N.

Linear correlation between DSSC efficiency, intramolecular charge transfer characteristics, and

NLO properties - DFT approach

Patil, M.

Stereocontrol through Synergistic Catalysis in the Enantioselective alpha-Alkenylation of Aldehyde: A Computational Study

Journal of Organic Chemistry, (83): 1304-1311. 2018. 10.1021/acs.joc.7b02822

Pavlova, A.; Parks, J. M.; Gumbart, J. C.

Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations

Journal of Chemical Theory and Computation, (14): 784-798. 2018. 10.1021/acs.jctc.7b01236

Pavlyukh, Y.; Rentschler, E.; Elmers, H. J.; Hubner, W.; Lefkidis, G.

Magnetism of metallacrown single-molecule magnets: From a simplest model to realistic systems

Physical Review B, (97) 2018. 10.1103/PhysRevB.97.214408

Payard, P. A.; Gu, Q. Y.; Guo, W. P.; Wang, Q. R.; Corbet, M.; Michel, C.; Sautet, P.; Grimaud, L.; Wischert, R.; Pera-Titus, M.

Direct Amination of Alcohols Catalyzed by Aluminum Triflate: AnExperimental and Computational Study

Chemistry-a European Journal, (24): 14146-14153. 2018. 10.1002/chem.201801492

Payard, P. A.; Perego, L. A.; Ciofini, I.; Grimaud, L.

Taming Nickel-Catalyzed Suzuki-Miyaura Coupling: A Mechanistic Focus on Boron-to-Nickel Transmetalation

ACS Catalysis, (8): 4812-4823. 2018. 10.1021/acscata1.8b00933

Payvand, A.; Tavangar, Z.

Computational study on the functionalization of BNNC with pyrrole molecule

Superlattices and Microstructures, (117): 373-381. 2018. 10.1016/j.spmi.2018.03.047

Pei, L.; Li, H. R.; Yan, M.; Chen, Q.; Mu, Y. W.; Lu, H. G.; Wu, Y. B.; Li, S. D.

Charge-induced structural transition between seashell-like B-29(-) and B-29(+) in 18 pi-electron configurations

Physical Chemistry Chemical Physics, (20): 15330-15334. 2018. 10.1039/c8cp01078a

Pembere, A. M. S.; Liu, X. H.; Ding, W. H.; Luo, Z. X.

How Partial Atomic Charges and Bonding Orbitals Affect the Reactivity of Aluminum Clusters with Water?

Journal of Physical Chemistry A, (122): 3107-3114. 2018. 10.1021/acs.jpca.7b10635

Penchoff, D. A.; Peterson, C. C.; Camden, J. P.; Bradshaw, J. A.; Auxier, J. D.; Schweitzer, G. K.; Jenkins, D. M.; Harrison, R. J.; Hall, H. L.

Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes

ACS Omega, (3): 13984-13993. 2018. 10.1021/acsomega.8b02068

Penchoff, D. A.; Peterson, C. C.; Quint, M. S.; Auxier, J. D.; Schweitzer, G. K.; Jenkins, D. M.; Harrison, R. J.; Hall, H. L.

Structural Characteristics, Population Analysis, and Binding Energies of An(No3) (2+) (with An = Ac to Lr)

ACS Omega, (3): 14127-14143. 2018. 10.1021/acsomega.8b01800

Pendas, A. M.; Francisco, E.

From quantum fragments to Lewis structures: electron counting in position space

Physical Chemistry Chemical Physics, (20): 21368-21380. 2018. 10.1039/c8cp04090g

Peng, H. L.; Huang, P. R.; Yi, P. G.; Xu, F.; Sun, L. X.

Theoretical studies of pi-electron delocalization and localization on intramolecular proton transfer in the ground state

Journal of Molecular Structure, (1154): 590-595. 2018. 10.1016/j.molstruc.2017.10.079

Perego, L. A.; Payard, P. A.; Haddou, B.; Ciofini, I.; Grimaud, L.

Evidence for a Cooperative Mechanism Involving Two Palladium(0) Centers in the Oxidative Addition of Iodoarenes

Chemistry-a European Journal, (24): 2192-2199. 2018. 10.1002/chem.201704899

Perils, J.; Cortezon-Tamarit, F.; Kuganathan, N.; Kociok-Kohn, G.; Dilworth, J. R.; Pascu, S. I.

Novel rhenium(V) nitride complexes with dithiocarbamate ligands - A synchrotron X-ray and DFT structural investigation

Inorganica Chimica Acta, (475): 142-149. 2018. 10.1016/j.ica.2017.11.023

Perotto, C. U.; Sodipo, C. L.; Jones, G. J.; Tidey, J. P.; Blake, A. J.; Lewis, W.; Davies, E. S.; McMaster, J.; Schroder, M.

Heterobimetallic NiFe Complexes Containing Mixed CO/CN- Ligands: Analogs of the Active Site of the NiFe Hydrogenases

Inorganic Chemistry, (57): 2558-2569. 2018. 10.1021/acs.inorgchem.7b02905

Philip, B. M.; John, J. S.; Kumar, K. M.; Devarajegowda, H. C.; Chandy, J.; Sajan, D.

Molecular docking and spectral analysis of (5,7-Dimethyl-2-oxo-2H-chromen-4-yl)-methyl diethyldithiocarbamate : A potential bioactive agent

Chemical Physics Letters, (711): 87-99. 2018. 10.1016/j.cplett.2018.09.033

Phung, Q. M.; Pierloot, K.

The dioxygen adducts of iron and manganese porphyrins: electronic structure and binding energy

Physical Chemistry Chemical Physics, (20): 17009-17019. 2018. 10.1039/c8cp03078b

Pichierri, F.

Adamantane template effect on the self-assembly of a molecular tetrahedron: A theoretical analysis

Chemical Physics Letters, (713): 149-152. 2018. 10.1016/j.cplett.2018.10.032

Pinheiro, P. D. M.; Rodrigues, D. A.; Alves, M. A.; Tinoco, L. W.; Ferreira, G. B.; de Sant'Anna, C. M. R.; Fraga, C. A. M.

Theoretical and experimental characterization of 1,4-N center dot center dot center dot S sigma-hole intramolecular interactions in bioactive N-acylhydrazone derivatives

New Journal of Chemistry, (42): 497-505. 2018. 10.1039/c7nj03543h

Pintus, A.; Aragoni, M. C.; Carcangiu, G.; Giacopetti, L.; Isaia, F.; Lippolis, V.; Maiore, L.; Meloni, P.; Arca, M.

Density functional theory modelling of protective agents for carbonate stones: a case study of oxalate and oxamate inorganic salts

New Journal of Chemistry, (42): 11593-11600. 2018. 10.1039/c8nj01714j

Piou, T.; Romanov-Michaelidis, F.; Ashley, M. A.; Romanova-Michaelides, M.; Rovis, T.

Stereodivergent Rhodium(III)-Catalyzed cis-Cyclopropanation Enabled by Multivariate Optimization

Journal of the American Chemical Society, (140): 9587-9593. 2018. 10.1021/jacs.8b04293

Pisano, P. L.; Espino, M.; Fernandez, M. D.; Silva, M. F.; Olivieri, A. C.

Structural analysis of natural deep eutectic solvents. Theoretical and experimental study  
Microchemical Journal, (143): 252-258. 2018. 10.1016/j.microc.2018.08.016

Pisano, P. L.; Pellegrinet, S. C.

Alkylhalovinylboranes: a new class of Diels-Alder dienophiles  
RSC Advances, (8): 33864-33871. 2018. 10.1039/c8ra07089j

Platts, J. A.; Baker, R. J.

Non-covalent interactions of uranyl complexes: a theoretical study

Physical Chemistry Chemical Physics, (20): 15380-15388. 2018. 10.1039/c8cp02444h

Pokhodnya, K.; Anderson, K.; Kilina, S.; Dandu, N.; Boudjouk, P.

Mechanism of Charged, Neutral, Mono-, and Polyatomic Donor Ligand Coordination to Perchlorinated Cyclohexasilane ( $\text{Si}_6\text{Cl}_{12}$ )

Journal of Physical Chemistry A, (122): 4067-4075. 2018. 10.1021/acs.jpca.7b11052

Polasek, M.; Makrlik, E.; Kvicala, J.; Krizova, V.; Vanura, P.

meso-Octamethylcalix 4 pyrrole as an effective macrocyclic receptor for the univalent thallium cation in the gas phase: Experimental and theoretical study

Journal of Molecular Structure, (1153): 78-84. 2018. 10.1016/j.molstruc.2017.09.103

Polyak, I.; Jenkins, A. J.; Vacher, M.; Bouduban, M. E. F.; Bearpark, M. J.; Robb, M. A.  
Charge migration engineered by localisation: electron-nuclear dynamics in polyenes and glycine  
*Molecular Physics*, (116): 2474-2489. 2018. 10.1080/00268976.2018.1478136

Pomelli, C. S.; Chiappe, C.  
A computational study of the effect of ionic liquid anions on Reichardt's dye solvatochromism  
*Theoretical Chemistry Accounts*, (137) 2018. 10.1007/s00214-018-2269-1

Pomogaev, V. A.; Ramazanov, R. R.; Ruud, K.; Artyukhov, V. Y.  
Insight into the fluorescence quenching of Trp214 at HSA by the Dimetridazole ligand from simulation  
*Journal of Photochemistry and Photobiology a-Chemistry*, (354): 86-100. 2018.  
10.1016/j.jphotochem.2017.08.041

Pomogaeva, A. V.; Scheer, M.; Timoshkin, A. Y.  
Why Do B-P and Al-P Polymers Differ? Structures, Stability, and Electronic Properties of Chain and Ring H<sub>2</sub>PEH<sub>2</sub> (n) Oligomers (E=B, Al; n=1-15)  
*Chemistry-a European Journal*, (24): 17046-17054. 2018. 10.1002/chem.201803008

Poor, M. A.; Darehkordi, A.; Anary-Abbasinejad, M.; Mohammadi, M.  
Gabapentin-base synthesis and theoretical studies of biologically active compounds: N-cyclohexyl-3-oxo-2-(3-oxo-2-azaspiro 4.5 decan-2-yl)-3-arylpropanamides and N-(tert-butyl)-2-(3-oxo-2-azaspiro 4.5 decan-2-yl)-2-arylacetamide derivatives  
*Journal of Molecular Structure*, (1152): 44-52. 2018. 10.1016/j.molstruc.2017.09.061

Poorsargol, M.; Delarami, H. S.  
A Quantum Chemical Study of Various Intramolecular Hydrogen Bonds in 4-Amino-3-Pentene-2-Thial  
*Journal of Structural Chemistry*, (59): 1276-1287. 2018. 10.1134/s0022476618060057

Popov, I. A.; Jimenez-Izal, E.; Alexandrova, A. N.; Boldyrev, A. I.  
Multicenter Bonding Effects in Oxygen Vacancy in the Bulk and on the Surface of MgO  
*Journal of Physical Chemistry C*, (122): 11933-11937. 2018. 10.1021/acs.jpcc.8b03118

Popov, I. A.; Starikova, A. A.; Steglenko, D. V.; Boldyrev, A. I.  
Usefulness of the sigma-Aromaticity and sigma-Antiaromaticity Concepts for Clusters and Solid-State Compounds  
*Chemistry-a European Journal*, (24): 292-+. 2018. 10.1002/chem.201702035

Possetto, D.; Natera, J.; Sancho, M. I.; Garcia, N. A.; Massad, W. A.  
Bioallethrin degradation by photo-Fenton process in acetonitrile/water and aqueous beta-cyclodextrin solutions

Journal of Photochemistry and Photobiology a-Chemistry, (365): 103-109. 2018.  
10.1016/j.jphotochem.2018.07.036

Postils, V.; Rodriguez, M.; Sabena, G.; Conde, A.; Diaz-Requejo, M. M.; Perez, P. J.; Costas, M.; Sola, M.; Luis, J. M.

Mechanism of the Selective Fe-Catalyzed Arene Carbon-Hydrogen Bond Functionalization  
ACS Catalysis, (8): 4313-4322. 2018. 10.1021/acscatal.7b03935

Pounraj, P.; Mohankumar, V.; Pandian, M. S.; Ramasamy, P.

Donor functionalized quinoline based organic sensitizers for dye sensitized solar cell (DSSC) applications: DFT and TD-DFT investigations

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3872-8

Prabhu, A. A. M.; Fatiha, M.; Leila, N.; Raj, T. A.; Navarro-Gonzalez, I.; Periago, M. J.; Yanez-Gascon, M. J.; Perez-Sanchez, H.

Investigation of 3D Contour Map and Intermolecular Interaction of Dopamine with beta-Cyclodextrin and 2-Hydroxypropyl-beta-cyclodextrin

Journal of Solution Chemistry, (47): 409-429. 2018. 10.1007/s10953-018-0728-x

Prakash, R.; De, A.; Kirubakaran, B.; Ghosh, S.

Metal-Rich Oxametallaboranes of Group 5 Metals: Synthesis and Structure of a Face-Fused mu(7)-Boride Cluster

Inorganic Chemistry, (57): 14748-14757. 2018. 10.1021/acs.inorgchem.8b02512

Prasertsab, A.; Maihom, T.; Probst, M.; Wattanakit, C.; Limtrakul, J.

Furfural to Furfuryl Alcohol: Computational Study of the Hydrogen Transfer on Lewis Acidic BEA Zeolites and Effects of Cation Exchange and Tetraivalent Metal Substitution

Inorganic Chemistry, (57): 6599-6605. 2018. 10.1021/acs.inorgchem.8b00741

Prashanth, J.; Reddy, B. V.

Study on structure, vibrational analysis and molecular characteristics of some halogen substituted azido-phenylethanones using FTIR spectra and DFT

Journal of Molecular Structure, (1155): 582-597. 2018. 10.1016/j.molstruc.2017.11.049

Prathap, K. N. C.; Lokanath, N. K.

Three novel coumarin-benzenesulfonylhydrazide hybrids: Synthesis, characterization, crystal structure, Hirshfeld surface, DFT and NBO studies

Journal of Molecular Structure, (1171): 564-577. 2018. 10.1016/j.molstruc.2018.06.022

Prathipa, C.; Kalpana, P.; Akilandeswari, L.

Role of hydrogen bonding in conformational energies of hexachlorophene and its derivatives - A theoretical study

Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (57): 643-648. 2018.

Proud, A. J.; Sheppard, B. J. H.; Pearson, J. K.

Revealing Electron-Electron Interactions within Lewis Pairs in Chemical Systems

Journal of the American Chemical Society, (140): 219-228. 2018. 10.1021/jacs.7b08935

Proud, A. J.; Sheppard, B. J. H.; Pearson, J. K.

Using the localized pair model to describe the nature of the hydrogen bond

Canadian Journal of Chemistry, (96): 681-688. 2018. 10.1139/cjc-2017-0677

Purkayastha, A.; Debnath, D.; Majumder, M.; Ortega-Castro, J.; Kirillov, A. M.; Ganguly, R.; Klak, J.; Frontera, A.; Misra, T. K.

Nickel(II) based homo- vs heterometallic 1D coordination polymers derived from a novel 6-aminouracil building block: Structures, topologies, non-covalent interactions, magnetism, and antibacterial activity

Inorganica Chimica Acta, (482): 384-394. 2018. 10.1016/j.ica.2018.06.037

Purushothaman, I.; De, S.; Parameswaran, P.

Different Donor-Acceptor Interactions of Carbene Ligands in Heteroleptic Divalent Group 14 Compounds, LEL' (E = C-Sn; L = N-Heterocyclic Carbene; L' = Cyclic Alkyl(Amino) Carbene)  
Chemistry-a European Journal, (24): 3816-3824. 2018. 10.1002/chem.201705719

Pusch, S.; Schollmeyer, D.; Opatz, T.

Synthesis and Unusual NMR-Spectroscopic Behavior of a Strained Bicyclic Ammonium Salt  
European Journal of Organic Chemistry: 1204-1207. 2018. 10.1002/ejoc.201701594

Pyles, D. A.; Coldren, W. H.; Eder, G.; Hadad, C. M.; McGrier, P. L.

Mechanistic investigations into the cyclization and crystallization of benzobisoxazole-linked two-dimensional covalent organic frameworks

Chemical Science, (9): 6417-6423. 2018. 10.1039/c8sc01683f

Qi, T.; Lyu, Y. J.; Wang, Z. M.; Yang, H. Q.; Hu, C. W.

Regular patterns of the effects of hydrogen-containing additives on the formation of CdSe monomer

Physical Chemistry Chemical Physics, (20): 20863-20873. 2018. 10.1039/c8cp02980f

Qian, M.; Qin, B. W.; Yuan, H. Y.; Li, W. L.; Zhang, J. P.

Mechanistic insights into N-Bromosuccinimide-promoted synthesis of imidazo 1,2-a pyridine in water: Reactivity mediated by substrates and solvent

Journal of Computational Chemistry, (39): 2324-2332. 2018. 10.1002/jcc.25564

Qin, Z. B.; Wang, H.; Ren, Y. D.; Zheng, X. F.; Cui, Z. F.; Tang, Z. C.

Electron velocity map imaging and theoretical study on CuXH (X=O and S) anions

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (188): 85-89. 2018.  
10.1016/j.saa.2017.06.039

Qin, Z. Z.; Wang, Q.; Yuan, C. X.; Yang, Y. T.; Zhao, X. F.; Li, D. B.; Liu, P.; Wu, Y. B.

Combining covalent bonding and electrostatic attraction to achieve highly viable species with ultrashort beryllium-beryllium distances: a computational design

Dalton Transactions, (47): 4707-4713. 2018. 10.1039/c7dt04897a

Qiu, S. Y.; Azofra, L. M.; MacFarlane, D. R.; Sun, C. H.

Hydrogen bonding effect between active site and protein environment on catalysis performance in H<sub>2</sub>-producing NiFe hydrogenases

Physical Chemistry Chemical Physics, (20): 6735-6743. 2018. 10.1039/c7cp07685a

Quan, J.; Shen, F. W.; Cai, H.; Zhang, Y. N.; Wu, H.

Galactose-Functionalized Double-Hydrophilic Block Glycopolymers and Their Thermoresponsive Self-Assembly Dynamics

Langmuir, (34): 10721-10731. 2018. 10.1021/acs.langmuir.8b01516

Quijano-Quinones, R. F.; Castro-Segura, C. S.; Mena-Rejon, G. J.; Quesadas-Rojas, M.; Caceres-Castillo, D.

Biosynthesis of Grandione: An Example of Tandem Hetero Diels-Alder/Retro-Claisen Rearrangement Reaction?

Molecules, (23) 2018. 10.3390/molecules23102505

Rajaraman, B. R.; Sheela, N. R.; Muthu, S.

Investigation on 1-Acetyl-4-(4-hydroxyphenyl) piperazine an anti fungal drug by spectroscopic, quantum chemical computations and molecular docking studies

Journal of Molecular Structure, (1173): 583-595. 2018. 10.1016/j.molstruc.2018.07.030

Rabanal-Leon, W. A.; Vasquez-Espinal, A.; Yanez, O.; Pino-Rios, R.; Arratia-Perez, R.; Alvarez-Thon, L.; Torres-Vega, J. J.; Tiznado, W.

Aromaticity of M-3(mu-X)(3)X-6 (0/2-) (M = Re and Tc, X = Cl, Br, I) Clusters Confirmed by Ring Current Analysis and Induced Magnetic Field

European Journal of Inorganic Chemistry: 3312-3319. 2018. 10.1002/ejic.201800339

Rachelin, Y. P.; Pradhan, S.; James, C.

Quantum chemical insight into molecular structure, density functional theory calculations, vibrational dynamics, natural population analysis, Hirshfeld analysis, and molecular docking approach to chalcone 1-4-bromophenyl-3-(2-methoxyphenyl)prop-2-en-1-one

Spectroscopy Letters, (51): 144-154. 2018. 10.1080/00387010.2018.1442352

Rad, A. S.; Aghaei, S. M.; Aali, E.; Peyravi, M.; Jahanshahi, M.

Application of chromium-doped fullerene as a carrier for thymine and uracil nucleotides: Comprehensive density functional theory calculations

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4070

Rad, A. S.; Aghaei, S. M.; Pazoki, H.; Binaeian, E.; Mirzaei, M.

Surface interaction of H<sub>2</sub>O and H<sub>2</sub>S onto Ca<sub>12</sub>O<sub>12</sub> nanocluster: Quantum-chemical analyses  
Surface and Interface Analysis, (50): 411-419. 2018. 10.1002/sia.6382

Rad, A. S.; Ayub, K.

How can nickel decoration affect H-2 adsorption on B<sub>12</sub>P<sub>12</sub> nano-heterostructures?

Journal of Molecular Liquids, (255): 168-175. 2018. 10.1016/j.molliq.2018.01.149

Rad, A. S.; Ayub, K.

Nonlinear optical, IR and orbital properties of Ni doped MgO nanoclusters: A DFT investigation  
Computational and Theoretical Chemistry, (1138): 39-47. 2018. 10.1016/j.comptc.2018.06.003

Radhika, R.; Shankar, R.; Vijayakumar, S.; Kolandaivel, P.

Role of 6-Mercaptopurine in the potential therapeutic targets DNA base pairs and G-quadruplex DNA: insights from quantum chemical and molecular dynamics simulations

Journal of Biomolecular Structure & Dynamics, (36): 1369-1401. 2018.

10.1080/07391102.2017.1323013

Radlow, M.; Czjzek, M.; Jeudy, A.; Dabin, J.; Delage, L.; Leblanc, C.; Hartung, J.

X-ray Diffraction and Density Functional Theory Provide Insight into Vanadate Binding to Homohexameric Bromoperoxidase II and the Mechanism of Bromide Oxidation

ACS Chemical Biology, (13): 1243-1259. 2018. 10.1021/acschembio.8b00041

Rafat, R.; Nowroozi, A.

A comprehensive theoretical study of conformational analysis, intramolecular hydrogen bond, pi-electron delocalization, and tautomeric preferences in 2-selenoformyl-3-thioxo-propionaldehyde

Structural Chemistry, (29): 1057-1065. 2018. 10.1007/s11224-018-1088-2

Rahim, A.; Sahariah, B.; Sarma, B. K.

N,N'-Di(acylamino)-2,5-diketopiperazines: Strategic Incorporation of Reciprocal n → pi\* Interactions in a Druglike Scaffold

Organic Letters, (20): 5743-5746. 2018. 10.1021/acs.orglett.8b02449

Rahimi, R.; Kamalinahad, S.; Solimannejad, M.

Adsorption of rare gases on the C-20 nanocage: a theoretical investigation

Materials Research Express, (5) 2018. 10.1088/2053-1591/aab0e3

Raikwar, M. M.; Rhyman, L.; Ramasami, P.; Sekar, N.

Theoretical Investigation of Difluoroboron Complex of Curcuminoid Derivatives with and without Phenyl Substituent (at Meso Position): Linear and Non-Linear Optical Study

Chemistryselect, (3): 11339-11349. 2018. 10.1002/slct.201802231

Raja, B.; Balachandran, V.; Revathi, B.; Anitha, K.

Structural study, NCA, FTIR, FT-Raman spectral investigations, NBO analysis and thermodynamic functions of N-benzyloxy carbonyl-L-alanine

Indian Journal of Pure & Applied Physics, (56): 509-521. 2018.

Rajaei, I.; Mirsattari, S. N.

Spectroscopic characteristic (FT-IR, H-1, C-13 NMR and UV-Vis) and theoretical calculations (MEP, DOS, HOMO-LUMO, PES, NBO analysis and keto-enol tautomerism) of new tetradentate N,N'-bis(4-hydroxysalicylidene)-1,4-phenylenediamine ligand as chelating agent for the synthesis of dinuclear Co(II), Ni(II), Cu(II) and Zn(II) complexes

Journal of Molecular Structure, (1163): 236-251. 2018. 10.1016/j.molstruc.2018.02.010

Rajagopalan, N. R.; Krishnamoorthy, P.; Jayamoorthy, K.

Experimental and Theoretical Investigations of Tetrakis (Thiourea) Palladium Chloride Semi-Organic Non-Linear Optical Crystal: An Approach to NLO Application

Silicon, (10): 841-850. 2018. 10.1007/s12633-016-9538-1

Rajan, R. V.; George, M.; Alex, J.; Sajan, D.; Vinitha, G.

Growth, effect of protonation and hydrogen bonding interactions of L-Histidine nitrate monohydrate, a potential semi organic third order nonlinear optical material

Optical Materials, (86): 198-212. 2018. 10.1016/j.optmat.2018.10.006

Rajan, V. K.; Ahamed, T. K. S.; Muraleedharan, K.

Studies on the UV filtering and radical scavenging capacity of the bitter masking flavanone Eriodictyol

Journal of Photochemistry and Photobiology B-Biology, (185): 254-261. 2018. 10.1016/j.jphotobiol.2018.06.017

Rajan, V. K.; Hasna, C. K.; Muraleedharan, K.

The natural food colorant Peonidin from cranberries as a potential radical scavenger - A DFT based mechanistic analysis

Food Chemistry, (262): 184-190. 2018. 10.1016/j.foodchem.2018.04.074

Rajeshwari, B.; Kalaiselvan, A.; Senthilnathan, D.

Ab initio and DFT investigations on the ring opening of aziridines using singlet unsaturated carbenes

Computational and Theoretical Chemistry, (1126): 1-6. 2018. 10.1016/j.comptc.2018.01.012

Ramachandran, K.; Vijayakumar, P.; Raja, A.; Mohankumar, V.; Vinitha, G.; Pandian, M. S.; Ramasamy, P.

Investigations on 4-methyl benzophenone (4MB) single crystal grown by Czochralski method and its characterization

Journal of Materials Science-Materials in Electronics, (29): 8571-8583. 2018. 10.1007/s10854-018-8871-0

Ramakrishnan, S.; Jemmis, E. D.

Origin of beta-agostic interaction in d(0) transition metal alkyl complexes: Influence of ligands

Journal of Organometallic Chemistry, (865): 37-44. 2018. 10.1016/j.jorganchem.2018.01.048

- Ramanan, R.; Danovich, D.; Mandal, D.; Shaik, S.  
Catalysis of Methyl Transfer Reactions by Oriented External Electric Fields: Are Gold-Thiolate Linkers Innocent?  
Journal of the American Chemical Society, (140): 4354-4362. 2018. 10.1021/jacs.8b00192
- Ramanathan, N.; Sarkar, S.; Sundararajan, K.; Chandrasekar, A.; Sankaran, K.; Suresh, A.  
Influence of Branching on the Conformational Space: Case Study of Tri-sec-butyl Phosphate Using Matrix Isolation Infrared Spectroscopy and DFT Computations  
Journal of Physical Chemistry A, (122): 8229-8242. 2018. 10.1021/acs.jpca.8b08157
- Ramasami, P.; Ford, T. A.  
An ab initio study of some binary complexes containing methyl fluoride and difluoromethane: red-shifting and blue-shifting hydrogen bonds  
Molecular Physics, (116): 1722-1736. 2018. 10.1080/00268976.2018.1445307
- Ramazani, A.; Sheikhi, M.; Hanifehpour, Y.; Asiabi, P. A.; Joo, S. W.  
Molecular Structure, Electronic Properties, Homo-Lumo, MEP and NBO Analysis of (N-Isocyanimino) Triphenylphosphorane (Ph<sub>3</sub>PNNC): DFT Calculations  
Journal of Structural Chemistry, (59): 529-540. 2018. 10.1134/s0022476618030058
- Ramesh, G.; Prashanth, J.; Naik, J. L.; Reddy, B. V.  
Molecular Structure, Vibrational Analysis, Hyperpolarizability and NBO Analysis of 3-Methyl-Picolinic Acid Using SQM Calculations  
Journal of Structural Chemistry, (59): 1022-1031. 2018. 10.1134/s0022476618050037
- Ramesh, G.; Reddy, B. V.  
Spectroscopic investigation on structure (monomer and dimer), molecular characteristics and comparative study on vibrational analysis of picolinic and isonicotinic acids using experimental and theoretical (DFT & IVP) methods  
Journal of Molecular Structure, (1160): 271-292. 2018. 10.1016/j.molstruc.2018.01.083
- Ramezanadeh, M.; Bahlakeh, G.; Sanaei, Z.; Ramezanadeh, B.  
Studying the *Urtica dioica* leaves extract inhibition effect on the mild steel corrosion in 1 M HCl solution: Complementary experimental, ab initio quantum mechanics, Monte Carlo and molecular dynamics studies  
Journal of Molecular Liquids, (272): 120-136. 2018. 10.1016/j.molliq.2018.09.059
- Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Fraut, J.  
A Systematic DFT Study of Some Plausible Zn(II) and Al(III) Interaction Sites in N-Terminally Acetylated alpha-Synuclein  
Journal of Physical Chemistry A, (122): 690-699. 2018. 10.1021/acs.jpca.7b10744
- Ramos, F.; Flores, H.; Hernandez-Perez, J. M.; Sandoval-Lira, J.; Camarillo, E. A.

The Intramolecular Hydrogen Bond N-H center dot center dot center dot S in 2,2'-Diaminodiphenyl Disulfide: Experimental and Computational Thermochemistry  
Journal of Physical Chemistry A, (122): 239-248. 2018. 10.1021/acs.jpca.7b08838

Rana, L. K.; Sharma, R.; Ahmed, B.; Kaur, D.; Kumar, S.; Hundal, G.; Mittal, S. K.  
Dicarboxamide polymorph derivatives for trace-level electrochemical sensing of Cu(II) supported with crystal structure and theoretical studies  
Analytical Methods, (10): 5643-5648. 2018. 10.1039/c8ay01967c

Rani, N.; Vikas  
Mechanism and Kinetics of the Gas-Phase Stereoinversion in Proteinogenic L-Threonine and Its Astrophysical Relevance  
Journal of Physical Chemistry A, (122): 7572-7586. 2018. 10.1021/acs.jpca.8b06659

Rani, V.; Boda, M.; Raju, S.; Patwari, G. N.; Singh, H. B.; Butcher, R. J.  
Synthesis and structure of arylselenium(II) and aryltellurium(II) cations based on rigid 5-tert-butyl-1,3-bis-(N-pentylbenzimidazol-2 '-yl)benzenes  
Dalton Transactions, (47): 9114-9127. 2018. 10.1039/c8dt01148f

Rashidi, H.; Ahmadpour, A.; Gholizadeh, M.; Bamoharram, F. F.; Moosavi, F.  
Effect of Magnetized Ethanol on the Shape Evolution of Zinc Oxide from Nanoparticles to Microrods: Experimental and Molecular Dynamic Simulation Study  
Advanced Powder Technology, (29): 349-358. 2018. 10.1016/j.apt.2017.11.022

Raugei, S.; Seefeldt, L. C.; Hoffman, B. M.  
Critical computational analysis illuminates the reductive-elimination mechanism that activates nitrogenase for N<sub>2</sub> reduction  
Proceedings of the National Academy of Sciences of the United States of America, (115): E10521-E10530. 2018. 10.1073/pnas.1810211115

Raut, A. H.; Costa, P.; Sander, W.  
Reactions of Arylcarbenes with Lewis Acids  
Chemistry-a European Journal, (24): 18043-18051. 2018. 10.1002/chem.201803695

Raveendra, M.; Chandrasekhar, M.; Reddy, K. C.; Venkatesulu, A.; Sivakumar, K.; Reddy, K. D.  
Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, H-1 NMR spectroscopic and DFT method  
Fluid Phase Equilibria, (462): 85-99. 2018. 10.1016/j.fluid.2018.01.025

Ravell, E.; Jalife, S.; Barroso, J.; Orozco-Ic, M.; Hernandez-Juarez, G.; Ortiz-Chi, F.; Pan, S.; Cabellos, J. L.; Merino, G.  
Structure and Bonding in CE5- (E=Al-Tl) Clusters: Planar Tetracoordinate Carbon versus Pentacoordinate Carbon

Chemistry-an Asian Journal, (13): 1467-1473. 2018. 10.1002/asia.201800261

Rawat, K. S.; Pathak, B.

Flexible proton-responsive ligand-based Mn(I) complexes for CO<sub>2</sub> hydrogenation: a DFT study  
Physical Chemistry Chemical Physics, (20): 12535-12542. 2018. 10.1039/c7cp08637g

Rawat, K. S.; Pathak, B.

The significance of acid-base properties in the key ligand for hydrogenation: role of amido ligand  
Journal of Chemical Sciences, (130) 2018. 10.1007/s12039-018-1477-5

Reddy, G. N.; Kumar, A. V.; Parida, R.; Chakraborty, A.; Giri, S.

Zintl superalkalis as building blocks of supersalts

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3806-5

Reddy, G. N.; Mukhopadhyay, A.; Parida, R.; Roymahapatra, G.; Giri, S.

Structure, bonding and superalkali behaviour of organo-Zintl clusters X<sub>7</sub>Me<sub>4</sub> (X = As, Sb and Bi)

Journal of the Indian Chemical Society, (95): 951-959. 2018.

Reddy, G. N.; Parida, R.; Chakraborty, A.; Giri, S.

Deltahedral Organo-Zintl Superhalogens

Chemistry-a European Journal, (24): 13654-13658. 2018. 10.1002/chem.201802713

Redondo, P.; Rayon, V. M.; Barrientos, C.; Largo, A.

Structural Trends in Monoboronyl Compounds: Analysis of the Interaction of Second-Row Elements with BO

Journal of Physical Chemistry A, (122): 398-409. 2018. 10.1021/acs.jpca.7b10482

Regiec, A.; Wojciechowski, P.; Pietraszko, A.; Maczynski, M.

Infrared spectra and other properties predictions of 5-amino-3-methyl-4-isoxazolecarbohydrazide with electric field simulation using CPC model

Journal of Molecular Structure, (1161): 320-338. 2018. 10.1016/j.molstruc.2018.01.085

Rehman, N.; Khalid, M.; Bhatti, M. H.; Yunus, U.; Braga, A. A. C.; Ahmed, F.; Ali Mashhadi, S. M.; Tahir, M. N.

Schiff base of isoniazid and ketoprofen: synthesis, X-ray crystallographic, spectroscopic, antioxidant, and computational studies

Turkish Journal of Chemistry, (42): 639-+. 2018. 10.3906/kim-1706-45

Reid, J. P.; Sigman, M. S.

Comparing quantitative prediction methods for the discovery of small-molecule chiral catalysts  
Nature Reviews Chemistry, (2): 290-305. 2018. 10.1038/s41570-018-0040-8

Reinhardt, C. R.; Hu, Q. H.; Bresnahan, C. G.; Hati, S.; Bhattacharyya, S.

Cyclic Changes in Active Site Polarization and Dynamics Drive the "Ping-pong" Kinetics in NRH:Quinone Oxidoreductase 2: An Insight from QM/MM Simulations  
ACS Catalysis, (8): 12015-12029. 2018. 10.1021/acscatal.8b04193

Reinhold, C. R. W.; Dong, Z. W.; Winkler, J. M.; Steinert, H.; Schmidtmann, M.; Muller, T.  
A One-Step Germole to Silole Transformation and a Stable Isomer of a Disilabenzene  
Chemistry-a European Journal, (24): 848-854. 2018. 10.1002/chem.201703955

Rengifo, E.; Gomez, S.; Arce, J. C.; Weinhold, F.; Restrepo, A.  
The role of hyperconjugation in the unusual conformation of thymine: A natural bond orbital analysis  
Computational and Theoretical Chemistry, (1130): 58-62. 2018. 10.1016/j.comptc.2018.03.005

Rey, A.; Ferao, A. E.; Streubel, R.  
Quantum Chemical Calculations on CHOP DerivativesSpanning the Chemical Space of Phosphinidenes, Phosphaketenes, Oxaphosphirennes, and COP- Isomers  
Molecules, (23) 2018. 10.3390/molecules23123341

Rezaeani, F.; Ghiasi, R.; Yousefi, M.  
Theoretical Studies of Solvent Effect on the Structure, Bonding, and Spectroscopic Properties (IR, NMR) in the cis- Pt(PH<sub>3</sub>)<sub>2</sub>(NCS)<sub>2</sub> and Pt(PH<sub>3</sub>)<sub>2</sub>(SCN)<sub>2</sub> Linkage Isomers  
Russian Journal of Physical Chemistry A, (92): 1748-1756. 2018. 10.1134/s0036024418090224

Rezaeian, M.; Izadyar, M.; Pour, A. N.  
Carbon Dioxide Absorption by the Imidazolium-Amino Acid Ionic Liquids, Kinetics, and Mechanism Approach  
Journal of Physical Chemistry A, (122): 5721-5729. 2018. 10.1021/acs.jpca.8b03152

Rezazadeh, M.; Ghiasi, R.; Jamehbozorgi, S.  
Influence of Solvent and Electric Field on the Structure and IR, P-31 NMR Spectroscopic Properties of a Titanocene-Benzyne Complex  
Journal of Applied Spectroscopy, (85): 526-534. 2018. 10.1007/s10812-018-0683-8

Rezazadeh, S.; Ebrahimi, A.  
A Computational Study on the Hydride Transfer Mechanism between Nicotinamide and Menadione  
Chemistryselect, (3): 11977-11985. 2018. 10.1002/slct.201802389

Ribeiro-Claro, P. J. A.; Vaz, P. D.; Nolasco, M. M.; Amado, A. M.  
Understanding the vibrational spectra of crystalline isoniazid: Raman, IR and INS spectroscopy and solid-state DFT study  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (204): 452-459. 2018. 10.1016/j.saa.2018.06.073

Rigamonti, L.; Forni, A.; Sironi, M.; Ponti, A.; Ferretti, A. M.; Baschieri, C.; Pasini, A.  
Experimental and theoretical investigations on magneto-structural correlation in trinuclear  
copper(II) hydroxido propellers  
*Polyhedron*, (145): 22-34. 2018. 10.1016/j.poly.2018.01.028

Rimola, A.; Skouteris, D.; Balucani, N.; Ceccarelli, C.; Enrique-Romero, J.; Taquet, V.; Ugliengo, P.  
Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective  
*ACS Earth and Space Chemistry*, (2): 720-734. 2018. 10.1021/acsearthspacechem.7b00156

Ringgold, M.; Rehe, D.; Hrobarik, P.; Kornienko, A. Y.; Emge, T. J.; Brennan, J. G.  
Thorium Cubanes-Synthesis, Solid-State and Solution Structures, Thermolysis, and Chalcogen  
Exchange Reactions  
*Inorganic Chemistry*, (57): 7129-7141. 2018. 10.1021/acs.inorgchem.8b00836

Rios-Gutierrez, M.; Nasri, L.; Nacereddine, A. K.; Djerourou, A.; Domingo, L. R.  
A molecular electron density theory study of the 3+2 cycloaddition reaction between an  
azomethine imine and electron deficient ethylenes  
*Journal of Physical Organic Chemistry*, (31) 2018. 10.1002/poc.3830

Rivera, A.; Uribe, J. M.; Rios-Motta, J.; Bolte, M.  
The Role of Hyperconjugation on the Structure and C-H Stretching Frequencies of 3,3-Ethane-  
1,2-diyl- bis-1,3,5-triazabicyclo 3.2.1 octane (ETABOC): An X-Ray Structure and Vibrational Study  
*Crystals*, (8) 2018. 10.3390/crust8060251

Rivera-Rivera, L. A.; McElmurry, B. A.; Scott, K. W.; Springer, S. D.; Lucchese, R. R.; Bevan, J. W.; Leonov,  
II; Coudert, L. H.  
6.2 mu m spectrum and 6-dimensional morphed potentials of OC-H2O  
*Chemical Physics*, (501): 35-45. 2018. 10.1016/j.chemphys.2017.11.003

Riyaz, M.; Goel, N.  
Computational design of boron doped lithium (BLin) cluster-based catalyst for N-2 fixation  
*Computational and Theoretical Chemistry*, (1130): 107-112. 2018.  
10.1016/j.comptc.2018.03.010

Riyaz, M.; Yadav, S.; Goel, N.  
Dispersion corrected density functional study of CO oxidation on pristine/functionalized/doped  
graphene surfaces in aqueous phase  
*Journal of Molecular Graphics & Modelling*, (79): 27-34. 2018. 10.1016/j.jmgm.2017.11.004

Rizwana, B. F.; Prasana, J. C.; Abraham, C. S.; Muthu, S.  
Spectroscopic investigation, hirshfeld surface analysis and molecular docking studies on anti-  
viral drug entecavir  
*Journal of Molecular Structure*, (1164): 447-458. 2018. 10.1016/j.molstruc.2018.03.090

Robles, A.; Franco-Perez, M.; Gazquez, J. L.; Cardenas, C.; Fuentealba, P.  
Local electrophilicity  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3785-6

Rocha, M.; Gil, D. M.; Echeverria, G. A.; Piro, O. E.; Jios, J. L.; Ulic, S. E.  
A new perfluoromethyl aminoenone derivative and the role of the hydrogen bonding in the intra- and intermolecular interactions  
Journal of Fluorine Chemistry, (208): 36-47. 2018. 10.1016/j.jfluchem.2018.01.001

Rogozhnikov, N. A.  
Interaction between Thallium and the Au(111) Surface. Quantum-Chemical Analysis  
Russian Journal of Electrochemistry, (54): 912-921. 2018. 10.1134/s1023193518130360

Rogozhnikov, N. A.  
Quantum-Chemical Study of the Adsorption of Bi<sup>3+</sup> Ions on Au(111)  
Russian Journal of Electrochemistry, (54): 1201-1208. 2018. 10.1134/s1023193518130372

Rogozhnikov, N. A.  
A Quantum-Chemical Study of the Adsorption of Pb Atoms on Au(111)  
Protection of Metals and Physical Chemistry of Surfaces, (54): 161-169. 2018.  
10.1134/s2070205118020119

Rohini; Baral, M.; Kanungo, B. K.  
Comparative studies of the electronic, binding and photophysical properties of a new nona-dentate hemi-cage tripodal HQ pendant trizaza-macrocycle with unfilled, half-filled and completely filled lanthanide ions  
New Journal of Chemistry, (42): 16040-16059. 2018. 10.1039/c8nj02217h

Romano, R. M.; Betancourt, A. M.; Della Vedova, C. O.; Zeng, X. Q.; Beckers, H.; Willner, H.; Schwabedissen, J.; Mitzel, N. W.  
Preparation and Properties of Chlorosulfuryl Chloroformate, ClC(O)OSO<sub>2</sub>Cl  
Inorganic Chemistry, (57): 14834-14842. 2018. 10.1021/acs.inorgchem.8b02581

Romanovic, M. C.; Milenkovic, M. R.; Pevec, A.; Turel, I.; Spasojevic, V.; Grubisic, S.; Radanovic, D.; Andelkovic, K.; Cobeljic, B.  
Crystal structures, magnetic properties and DFT study of cobalt(II) azido complexes with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent  
Polyhedron, (139): 142-147. 2018. 10.1016/j.poly.2017.10.018

Romero-Fernandez, M. P.; Babiano, R.; Cintas, P.  
On the asymmetric autocatalysis of aldol reactions: The case of 4-nitrobenzaldehyde and acetone. A critical appraisal with a focus on theory  
Chirality, (30): 445-456. 2018. 10.1002/chir.22805

Roohi, H.; Alizadeh, P.  
Fine tuning the emission wavelengths of the 7-hydroxy-1-indanone based nano-structure dyes:  
Near-infrared (NIR) dual emission generation with large stokes shifts  
*Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy*, (196): 83-102. 2018.  
10.1016/j.saa.2018.01.081

Roohi, H.; Nokhostin, R.  
Molecular engineering of the photo switching in the ortho chromophores of the nanostructured green fluorescence protein  
*Journal of Luminescence*, (196): 406-424. 2018. 10.1016/j.jlumin.2017.12.056

Roohi, H.; Salehi, R.  
Molecular engineering of the electronic, structural, and electrochemical properties of nanostructured 1-methyl-4-phenyl 1,2,4 triazolium-based PhMTZ X1-10 ionic liquids through anionic changing  
*Ionics*, (24): 483-504. 2018. 10.1007/s11581-017-2198-3

Roohi, H.; Sherkhani, H. R.; Mahboub, H.  
Fine-tuning the photophysical properties of the five quinolin based nanophotowithes in the gas phase, polar and nonpolar solvents: A TD-DFT approach  
*Journal of Luminescence*, (204): 230-243. 2018. 10.1016/j.jlumin.2018.08.019

Rosenberg, R. E.  
The Strength of Hydrogen Bonds between Fluoro-Organics and Alcohols, a Theoretical Study  
*Journal of Physical Chemistry A*, (122): 4521-4529. 2018. 10.1021/acs.jpca.8b01148

Rosener, T.; Hoffmann, A.; Herres-Pawlis, S.  
Next Generation of Guanidine Quinoline Copper Complexes for Highly Controlled ATRP:  
Influence of Backbone Substitution on Redox Chemistry and Solubility  
*European Journal of Inorganic Chemistry*: 3164-3175. 2018. 10.1002/ejic.201800511

Roston, D.; Lu, X. Y.; Fang, D.; Demapan, D.; Cui, Q.  
Analysis of Phosphoryl-Transfer Enzymes with QM/MM Free Energy Simulations  
*Phosphatases*, (607): 53-90. 2018. 10.1016/bs.mie.2018.05.005

Rouhani, M.  
Full structural analysis of steviol: A DFT study  
*Journal of Molecular Structure*, (1173): 679-689. 2018. 10.1016/j.molstruc.2018.07.029

Rovaletti, A.; Greco, C.  
Organophosphorous ligands in hydrogenase-inspired iron-based catalysts: A DFT study on the energetics of metal protonation as a function of P-atom substitution  
*Journal of Physical Organic Chemistry*, (31) 2018. 10.1002/poc.3748

Roy, R. S.; Nandi, P. K.

Electronic structure and large second-order non-linear optical property of COT derivatives - a theoretical exploration

Physical Chemistry Chemical Physics, (20): 18744-18755. 2018. 10.1039/c8cp00163d

Roy, S.; Bohme, M.; Dash, S. P.; Mohanty, M.; Buchholz, A.; Plass, W.; Majumder, S.; Kulanthaivel, S.; Banerjee, I.; Reuter, H.; Kaminsky, W.; Dinda, R.

Anionic Dinuclear Oxidovanadium(IV) Complexes with Azo Functionalized Tridentate Ligands and mu-Ethoxido Bridge Leading to an Unsymmetric Twisted Arrangement: Synthesis, X-ray Structure, Magnetic Properties, and Cytotoxicity

Inorganic Chemistry, (57): 5767-5781. 2018. 10.1021/acs.inorgchem.8b00035

Roychoudhury, S.; O'Regan, D. D.; Sanvito, S.

Wannier-function-based constrained DFT with nonorthogonality-correcting Pulay forces in application to the reorganization effects in graphene-adsorbed pentacene

Physical Review B, (97) 2018. 10.1103/PhysRevB.97.205120

Ruccolo, S.; Rauch, M.; Parkin, G.

Synthesis and Structural Characterization of Tris(isopropylbenzimidazol-2-ylthio)methyl Zinc Complexes, Titm(PriBenz) ZnX: Modulation of Transannular Zn-C Interactions

Organometallics, (37): 1708-1718. 2018. 10.1021/acs.organomet.8b00158

Ruf, A.; Kanawati, B.; Schmitt-Kopplin, P.

Do dihydroxymagnesium carboxylates form Grignard-type reagents? A theoretical investigation on decarboxylative fragmentation

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3639-2

Rugg, G.; Genest, A.; Rosch, N.

DFT Variants for Mixed-Metal Oxides. Benchmarks Using Multi-Center Cluster Models

Journal of Physical Chemistry A, (122): 7042-7050. 2018. 10.1021/acs.jpca.8b05331

Ruiperez, F.; Galdeano, M.; Gimenez, E.; Matxain, J. M.

Sulfenamides as Building Blocks for Efficient Disulfide-Based Self-Healing Materials. A Quantum Chemical Study

Chemistryopen, (7): 248-255. 2018. 10.1002/open.201800003

Rumyantsev, M.; Kazantsev, O. A.; Rumyantsev, S.; Kalagaev, I. Y.

Quantum chemical study of the impact of protective association on the chemoselective synthesis of carboxybetaine from 2-(dimethylamino) ethanol and acrylic acid

Computational and Theoretical Chemistry, (1129): 16-25. 2018. 10.1016/j.comptc.2018.02.017

Rumyantsev, M.; Rumyantsev, S.

Combining advantages of homogeneous organocatalysis and heterogeneous catalysis with thermosensitive single-chain nanoparticles in a representative tetrahydropyranilation of alcohols

Polymer, (136): 101-108. 2018. 10.1016/j.polymer.2017.12.058

Rumyantsev, M.; Rumyantsev, S.; Kalagaev, I. Y.

Effect of Water on the Activation Thermodynamics of Deep Eutectic Solvents Based on Carboxybетaine and Choline

Journal of Physical Chemistry B, (122): 5951-5960. 2018. 10.1021/acs.jpcb.8b01218

Rungnim, C.; Faungnawakij, K.; Sano, N.; Kungwan, N.; Namuangruk, S.

Hydrogen storage performance of platinum supported carbon nanohorns: A DFT study of reaction mechanisms, thermodynamics, and kinetics

International Journal of Hydrogen Energy, (43): 23336-23345. 2018.

10.1016/j.ijhydene.2018.10.211

Rungthanaphatsophon, P.; Huang, P.; Walensky, J. R.

Phosphorano-Stabilized Carbene Complexes with Short Thorium(IV)- and Uranium(IV)-Carbon Bonds

Organometallics, (37): 1884-1891. 2018. 10.1021/acs.organomet.8b00137

Ruttert, M.; Holtstiege, F.; Husker, J.; Borner, M.; Winter, M.; Placke, T.

Hydrothermal-derived carbon as a stabilizing matrix for improved cycling performance of silicon-based anodes for lithium-ion full cells

Beilstein Journal of Nanotechnology, (9): 2381-2395. 2018. 10.3762/bjnano.9.223

Ryazantsev, S. V.; Lundell, J.; Feldman, V. I.; Khriachtchev, L.

Photochemistry of the H<sub>2</sub>O/CO System Revisited: The HXeOH center dot center dot center dot CO Complex in a Xenon Matrix

Journal of Physical Chemistry A, (122): 159-166. 2018. 10.1021/acs.jpca.7b10293

Rybacka, O.; Brzeski, J.; Anusiewicz, I.; Skurski, P.

The acid strength of the datively bound complexes involving AlF<sub>3</sub> lone pair acceptor and various lone pair donors

Chemical Physics Letters, (706): 488-493. 2018. 10.1016/j.cplett.2018.06.059

Rybacka, O.; Skurski, P.

Mechanism of the ethanol-based (C<sub>2</sub>H<sub>5</sub>OH<sub>2</sub>)<sup>(+)</sup>(SbF<sub>6</sub>)<sup>(-)</sup> salt formation by the superacid-catalyzed acetaldehyde hydrogenation

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2312-2

Sa, E. D.; Rodriguez-Santiago, L.; Sodupe, M.; Solans-Monfort, X.

Influence of Ligands and Oxidation State on the Reactivity of Pentacoordinated Iron Carbenes with Olefins: Metathesis versus Cyclopropanation

Organometallics, (37): 1229-1241. 2018. 10.1021/acs.organomet.7b00786

Saadat, K.; Shiri, A.; Kovacevic, B.

Substituted troponimines: when aromatization of the conjugate acid leads to very strong neutral organic superbases

New Journal of Chemistry, (42): 14568-14575. 2018. 10.1039/c8nj02349b

Sabaqian, S.; Nemati, F.; Nahzomi, H. T.; Heravi, M. M.

Silver(I) dithiocarbamate on modified magnetic cellulose: Synthesis, density functional theory study and application

Carbohydrate Polymers, (184): 221-230. 2018. 10.1016/j.carbpol.2017.12.045

Sabet-Sarvestani, H.; Izadyar, M.; Eshghi, H.; Noroozi-Shad, N.

Understanding the thermodynamic and kinetic performances of the substituted phosphorus ylides as a new class of compounds in carbon dioxide activation

Energy, (145): 329-337. 2018. 10.1016/j.energy.2017.12.149

Sabet-Sarvestani, H.; Izadyar, M.; Eshghi, H.; Noroozi-Shad, N.; Bakavoli, M.

Proton sponge as a new efficient catalyst for carbon dioxide transformation to methanol: Theoretical approach

Fuel, (221): 491-500. 2018. 10.1016/j.fuel.2018.02.094

Sabounchei, S. J.; Hashemi, A.; Sayadi, M.; Bayat, M.; Sedghi, A.; Karamian, R.; Farida, S. H. M.; Gable, R. W.

New highly soluble 6,6 -methanofullerene derivatives incorporating both alpha-keto and alpha, beta-ester stabilized phosphorus ylides; synthesis, characterization, theoretical and biological studies

Journal of Molecular Structure, (1165): 142-152. 2018. 10.1016/j.molstruc.2018.03.124

Sadhu, B.; Mishra, V.

The coordination chemistry of lanthanide and actinide metal ions with hydroxypyridinone-based decorporation agents: orbital and density based analyses

Dalton Transactions, (47): 16603-16615. 2018. 10.1039/c8dt03262a

Saeed, A.; Arif, M.; Erben, M. F.; Florke, U.; Simpson, J.

One-pot synthesis, quantum chemical calculations and X-ray diffraction studies of thiazolyl-coumarin hybrid compounds

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (198): 290-296. 2018. 10.1016/j.saa.2018.03.036

Safaei, Z.; Shiroudi, A.; Padash, R.; Sillanpaa, M.; Zahedi, E.

Reaction mechanisms and kinetics of the beta-elimination processes of compounds CHF<sub>2</sub>CH<sub>2</sub>SiFnMe<sub>3-n</sub> (n=0-3): DFT and CBS-QB3 methods using Rice-Ramsperger-Kassel-Marcus and transition state theories

Journal of Fluorine Chemistry, (216): 71-80. 2018. 10.1016/j.jfluchem.2018.10.009

Safdari, F.; Shamkhali, A. N.; Tafazzoli, M.; Parsafar, G.

Adsorption of pollutant cations from their aqueous solutions on graphitic carbon nitride explored by density functional theory

Journal of Molecular Liquids, (260): 423-435. 2018. 10.1016/j.molliq.2018.03.114

Sagdinc, S. G.; Azkeskin, C.; Esme, A.

Theoretical and spectroscopic studies of a tricyclic antidepressant, imipramine hydrochloride

Journal of Molecular Structure, (1161): 169-184. 2018. 10.1016/j.molstruc.2018.02.056

Sah, C.; Yadav, A. K.; Venkataramani, S.

Deciphering Stability of Five-Membered Heterocyclic Radicals: Balancing Act Between Delocalization and Ring Strain

Journal of Physical Chemistry A, (122): 5464-5476. 2018. 10.1021/acs.jpca.8b03145

Saha, B.; Bhattacharyya, P. K.

Density Functional Study on the Adsorption of 5-Membered N-Heterocycles on B/N/BN-Doped Graphene: Coronene as a Model System

ACS Omega, (3): 16753-16768. 2018. 10.1021/acsomega.8b02340

Saha, K.; Kar, S.; Ghosh, S.

Chalcogen stabilized cubane-type cluster: Synthesis and structure of  $(Cp^*Ta)(3)(\mu-Se)(3)(\mu(3)-Se)(3)B(OBuCl)$

Journal of the Indian Chemical Society, (95): 729-734. 2018.

Saha, R.; Chattaraj, P. K.

Activation of Small Molecules (H<sub>2</sub>, CO<sub>2</sub>, N<sub>2</sub>O, CH<sub>4</sub>, and C<sub>6</sub>H<sub>6</sub>) by a Porphyrinoid-Based Dimagnesium(I) Complex, an Electride

ACS Omega, (3): 17199-17211. 2018. 10.1021/acsomega.8b03006

Saha, R.; Mandal, B.; Chattaraj, P. K.

HN<sub>g</sub>BeF(3) (Ng=Ar-Rn): Superhalogen-supported noble gas insertion compounds  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25499

Saha, R.; Pan, S.; Chattaraj, P. K.

Stabilization of Boron-Boron Triple Bonds by Mesoionic Carbenes

ACS Omega, (3): 13720-13730. 2018. 10.1021/acsomega.8b02305

Sahadevan, S. A.; Cadoni, E.; Monni, N.; de Pipaon, C. S.; Mascaros, J. R. G.; Abherve, A.; Avarvari, N.; Marchio, L.; Arca, M.; Mercuri, M. L.

Structural Diversity in a New Series of Halogenated Quinolyl Salicylaldimides-Based Fe-III Complexes Showing Solid-State Halogen-Bonding/Halogen center dot center dot center dot Halogen Interactions

Crystal Growth & Design, (18): 4187-4199. 2018. 10.1021/acs.cgd.8b00753

Sajjad, M. A.; Harrison, J. A.; Nielson, A. J.

NBO Orbital Interaction Analysis for the Ambiphilic Metal-Ligand Activation/Concerted Metalation Deprotonation (AMLA/CMD) Mechanism Involved in the Cyclopalladation Reaction of N,N-Dimethylbenzylamine with Palladium Acetate

Organometallics, (37): 3659-3669. 2018. 10.1021/acs.organomet.8b00303

Sajjad, M. A.; Schwerdtfeger, P.; Harrison, J. A.; Nielson, A. J.

Electronic manipulation of the agostic and syndetic components in 1-tetralone oxime and imine complexes of palladium (II)

Polyhedron, (151): 66-73. 2018. 10.1016/j.poly.2018.05.025

Sakata, K.

Force constant decomposition for penta-coordinated XH<sub>3</sub>Cl<sub>2</sub>- (X=C, Si, Ge) structures

Journal of Computational Chemistry, (39): 1544-1550. 2018. 10.1002/jcc.25226

Sakthivel, S.; Alagesan, T.; Muthu, S.; Abraham, C. S.; Geetha, E.

Quantum mechanical, spectroscopic study (FT-IR and FT - Raman), NBO analysis, HOMO-LUMO, first order hyperpolarizability and docking studies of a non-steroidal anti-inflammatory compound

Journal of Molecular Structure, (1156): 645-656. 2018. 10.1016/j.molstruc.2017.12.024

Sala, D.; Musiani, F.; Rosato, A.

Application of Molecular Dynamics to the Investigation of Metalloproteins Involved in Metal Homeostasis

European Journal of Inorganic Chemistry: 4661-4677. 2018. 10.1002/ejic.201800602

Salehi, M.; Heidari, Z.; Omidyan, R.

Photophysics of Protonated and Microhydrated 2-Aminobenzaldehyde: Theoretical Insights into Photoswitchability of Protonated Systems

Journal of Physical Chemistry A, (122): 8849-8857. 2018. 10.1021/acs.jpca.8b09930

Salehzadeh, S.; Maleki, F.

Where and How Does an Organic Molecule Having a C-X Bond Release X- Anion Like an Inorganic Compound? A Theoretical Study

Journal of Physical Chemistry A, (122): 7598-7613. 2018. 10.1021/acs.jpca.8b07238

Salome, K. S.; Tormena, C. F.

Revisiting the Long-Range Perlin Effect in a Conformationally Constrained Oxocane

Journal of Organic Chemistry, (83): 10501-10504. 2018. 10.1021/acs.joc.8b00935

Salpin, J. Y.; Latrous, L.; Haldys, V.; Lamsabhi, A.

Interactions of Dimethyltin(IV) with Uracil As Studied in the Gas Phase

Journal of Physical Chemistry A, (122): 992-1003. 2018. 10.1021/acs.jpca.7b11510

Samanta, B.; Sengupta, T.; Pal, S.

Specificity of Amino Acid-Aluminum Cluster Interaction and Subsequent Oxygen Activation by the above Complex

Journal of Physical Chemistry C, (122): 28310-28323. 2018. 10.1021/acs.jpcc.8b08396

Samiee, S.; Taghvaeian, S.

The role of metals and dithiolate ligands on structural, electronic and optical properties of M(bipyridine)(dithiolate) complexes: A theoretical study

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (198): 150-159. 2018. 10.1016/j.saa.2018.03.010

San Fabian, J.; Omar, S.; de la Vega, J. M. G.

Transmission of the spin-spin coupling constants through hydrogen bonds in ammonia clusters European Physical Journal B, (91) 2018. 10.1140/epjb/e2018-90118-5

Sanchez-Marquez, J.; Zorrilla, D.; Garcia, V.; Fernandez, M.

Introducing a new bond reactivity index: Philicities for natural bond orbitals

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-017-3553-z

Sanchez-Marquez, J.; Zorrilla, D.; Garcia, V.; Fernandez, M.

Introducing a new methodology for the calculation of local philicity and multiphilic descriptor: an alternative to the finite difference approximation

Molecular Physics, (116): 1737-1748. 2018. 10.1080/00268976.2018.1445875

Sanchez-Sanz, G.; Crowe, D.; Nicholson, A.; Fleming, A.; Carey, E.; Kelleher, F.

Conformational studies of Gram-negative bacterial quorum sensing acyl homoserine lactone (AHL) molecules: The importance of the n → π\* interaction

Biophysical Chemistry, (238): 16-21. 2018. 10.1016/j.bpc.2018.04.002

Sanchez-Sanz, G.; Trujillo, C.

Improvement of Anion Transport Systems by Modulation of Chalcogen Interactions: The influence of solvent

Journal of Physical Chemistry A, (122): 1369-1377. 2018. 10.1021/acs.jpca.7b10920

Sangari, M. S.; Haghghi, M. G.; Nabavizadeh, S. M.; Pfitzner, A.; Rashidi, M.

Influence of ancillary ligands on the photophysical properties of cyclometalated organoplatinum( II) complexes

New Journal of Chemistry, (42): 8661-8671. 2018. 10.1039/c7nj04888b

Sanusi, Z. K.; Govender, T.; Maguire, G. E. M.; Maseko, S. B.; Lin, J.; Kruger, H. G.; Honarpasvar, B.

An insight to the molecular interactions of the FDA approved HIV PR drugs against L38L up arrow N up arrow L PR mutant

Journal of Computer-Aided Molecular Design, (32): 459-471. 2018. 10.1007/s10822-018-0099-9

Sanz, P.; Montero-Campillo, M. M.; Mo, O.; Yanez, M.; Alkorta, I.; Elguero, J.

Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2274-4

Sao, S.; Naskar, S.; Mukhopadhyay, N.; Das, M.; Chaudhuri, D.

Assisted pi-stacking: a strong synergy between weak interactions

Chemical Communications, (54): 12186-12189. 2018. 10.1039/c8cc07207h

Saraf, S. H.; Ghiasi, R.

Theoretical exploring of the substituent effect on the NQR and NMR parameters in a platinum-based anticancer drug, trans-(NHC) PtI<sub>2</sub> (para-NC<sub>5</sub>H<sub>4</sub>X) complex

Structural Chemistry, (29): 435-440. 2018. 10.1007/s11224-017-1040-x

Saraswat, M.; Venkataramani, S.

Through bond and through space interactions in dehydro-diazine radicals: a case study of 3c-5e interactions

Physical Chemistry Chemical Physics, (20): 4386-4395. 2018. 10.1039/c7cp07579k

Sarhadinia, S.; Ebrahimi, A.

The effect of anion-pi interactions on the properties of pyrazinamide and some related compounds

Computational and Theoretical Chemistry, (1124): 51-58. 2018. 10.1016/j.comptc.2017.12.003

Sarkar, R.; Kundu, T. K.

Density functional theory studies on PVDF/ionic liquid composite systems

Journal of Chemical Sciences, (130) 2018. 10.1007/s12039-018-1522-4

Sarkar, S.; Ramanathan, N.; Sundararaian, K.

Effect of Methyl Substitution on the N-H center dot center dot center dot O Interaction in Complexes of Pyrrole with Water, Methanol, and Dimethyl Ether: Matrix Isolation Infrared Spectroscopy and ab Initio Computational Studies

Journal of Physical Chemistry A, (122): 2445-2460. 2018. 10.1021/acs.jpca.8b00023

Sarkar, S.; Ramanathan, N.; Sundararajan, K.

Experimental Evidence of Synergistic Interactions in Pyrrole-Phenol Complexes at Low Temperatures under Isolated Conditions

Journal of Physical Chemistry A, (122): 9073-9083. 2018. 10.1021/acs.jpca.8b09076

Sarnowski, M. P.; Pedretty, K. P.; Giddings, N.; Woodcock, H. L.; Del Valle, J. R.

Synthesis and beta-sheet propensity of constrained N-amino peptides

Bioorganic & Medicinal Chemistry, (26): 1162-1166. 2018. 10.1016/j.bmc.2017.08.017

Sas, E. B.; Cankaya, N.; Kurt, M.

Synthesis of 2-(bis(cyanomethyl)amino)-2-oxoethyl methacrylate monomer molecule and its characterization by experimental and theoretical methods

Journal of Molecular Structure, (1161): 433-441. 2018. 10.1016/j.molstruc.2018.01.088

Sasi, B. S. A.; Alen, S.; Joy, L. K.; Sajan, D.; James, C.

Study on growth, electronic structure, topological and nonlinear optical properties of semi organic material sodium sulfanilate dehydrate

Journal of Materials Science-Materials in Electronics, (29): 17887-17902. 2018. 10.1007/s10854-018-9904-4

Saswati; Adao, P.; Majumder, S.; Dash, S. P.; Roy, S.; Kuznetsov, M. L.; Pessoa, J. C.; Gomes, C. S. B.; Hardikar, M. R.; Tiekkink, E. R. T.; Dinda, R.

Synthesis, structure, solution behavior, reactivity and biological evaluation of oxidovanadium(IV/V) thiosemicarbazone complexes

Dalton Transactions, (47): 11358-11374. 2018. 10.1039/c8dt01668b

Sathish, M.; Meenakshi, G.; Xavier, S.; Sebastian, S.; Periandy, S.; Ahmad, N.; Jamalis, J.; Rosli, M.; Fun, H. K.

Synthesis, molecular structure, Hirshfeld surface, spectral investigations and molecular docking study of 3-(5-bromo-2-thieny1)-1-(4-fluoropheny1)-3-acetyl-2-pyrazoline (2) by DFT method

Journal of Molecular Structure, (1164): 420-437. 2018. 10.1016/j.molstruc.2018.03.004

Sathya, K.; Dhamodharan, P.; Dhandapani, M.

Hydrogen bonded 2-methyl-1H-imidazol-3-ium 3,5-dinitrobenzoate 3,5-dinitrobenzoic acid, a new optical crystal: Evaluation of properties by structural, spectral, quantum chemical calculations, Z-scan and Hirshfeld studies

Journal of Physics and Chemistry of Solids, (114): 228-239. 2018. 10.1016/j.jpcs.2017.10.036

Sathya, K.; Dhamodharan, P.; Dhandapani, M.

Spectral, optical, thermal, Hirshfeld analysis and computational calculations of a new organic proton transfer crystal, 1H-benzo d 1,2,3 triazol-3-ium-3,5-dinitrobenzoate

Journal of Physics and Chemistry of Solids, (116): 281-291. 2018. 10.1016/j.jpcs.2018.01.040

Sathya, K.; Dhamodharan, P.; Dhandapani, M.

Structural characterization and DFT study of a new optical crystal: 2-amino-3-methylpyridinium-3,5-dinitrobenzoate

Optics and Laser Technology, (101): 328-340. 2018. 10.1016/j.optlastec.2017.11.027

Savastano, M.; Garcia, C.; de la Torre, M. D. L.; Pichierri, F.; Bazzicalupi, C.; Bianchi, A.; Melguizo, M.

Interplay between salt bridge, hydrogen bond and anion-pi interactions in thiocyanate binding Inorganica Chimica Acta, (470): 133-138. 2018. 10.1016/j.ica.2017.04.029

Scheiner, S.

Steric Crowding in Tetrel Bonds

Journal of Physical Chemistry A, (122): 2550-2562. 2018. 10.1021/acs.jpca.7b12357

Scheiner, S.; Lu, J.

Halogen, Chalcogen, and Pnicogen Bonding Involving Hypervalent Atoms  
Chemistry-a European Journal, (24): 8167-8177. 2018. 10.1002/chem.201800511

Schmid, M. H.; Das, A. K.; Landis, C. R.; Meuwly, M.

Multi-State VALBOND for Atomistic Simulations of Hypervalent Molecules, Metal Complexes, and Reactions

Journal of Chemical Theory and Computation, (14): 3565-3578. 2018. 10.1021/acs.jctc.7b01210

Schneider, C.; LaFortune, J. H. W.; Melen, R. L.; Stephan, D. W.

Lewis and Bronsted basicity of phosphine-diazomethane derivatives  
Dalton Transactions, (47): 12742-12749. 2018. 10.1039/c8dt02420k

Schneider, F. S. S.; Caramori, G. F.; Parreira, R. L. T.; Lippolis, V.; Arca, M.; Ciancaleoni, G.

Bond Analysis in Dihalogen-Halide and Dihalogen-Dimethylchalcogenide Systems  
European Journal of Inorganic Chemistry: 1007-1015. 2018. 10.1002/ejic.201701337

Schneider, F. S. S.; Segala, M.; Caramori, G. F.; da Silva, E. H.; Parreira, R. L. T.; Schrekker, H. S.; van Leeuwen, P.

How Do Secondary Phosphine Oxides Interact with Silver Nanoclusters? Insights from Computation

Journal of Physical Chemistry C, (122): 21449-21461. 2018. 10.1021/acs.jpcc.8b06244

Schrempp, D. F.; Kaifer, E.; Himmel, H. J.

Solvent Control of Ligand-Metal Electron Transfer in Mononuclear Copper Complexes with Redox-Active Bisguanidine Ligands

European Journal of Inorganic Chemistry: 3660-3667. 2018. 10.1002/ejic.201800525

Schulz, A.

Group 15 biradicals: synthesis and reactivity of cyclobutane-1,3-diyl and cyclopentane-1,3-diyl analogues

Dalton Transactions, (47): 12827-12837. 2018. 10.1039/c8dt03038c

Schutt, O.; VandeVondele, J.

Machine Learning Adaptive Basis Sets for Efficient Large Scale Density Functional Theory Simulation

Journal of Chemical Theory and Computation, (14): 4168-4175. 2018. 10.1021/acs.jctc.8b00378

Sebesta, F.; Baxova, K.; Burda, J. V.

Redox Potentials for Tetraplatin, Satraplatin, Its Derivatives, and Ascorbic Acid: A Computational Study

Inorganic Chemistry, (57): 951-962. 2018. 10.1021/acs.inorgchem.7b01894

- Sebesta, F.; Burda, J. V.  
Interactions of Ascorbic Acid with Satraplatin and its trans Analog JM576: DFT Computational Study  
European Journal of Inorganic Chemistry: 1481-1491. 2018. 10.1002/ejic.201701334
- Sedghamiz, E.; Khashei, F.; Moosavi, M.  
Linear tricationic ionic liquids: Insights into the structural features using DFT and molecular dynamics simulation  
Journal of Molecular Liquids, (271): 96-104. 2018. 10.1016/j.molliq.2018.08.111
- Sedghamiz, T.; Ghalami, F.; Sedghamiz, E.; Bahrami, M.  
Chiral recognition of propranolol enantiomers by chiral ionic liquid: A quantum chemical calculation analysis  
Computational and Theoretical Chemistry, (1140): 38-48. 2018. 10.1016/j.comptc.2018.07.017
- Selimovic, E.; Jeremic, S.; Licina, B.; Soldatovic, T.  
Kinetics, DFT Study and Antibacterial Activity of Zinc(II) and Copper(II) Terpyridine Complexes  
Journal of the Mexican Chemical Society, (62) 2018.
- Selmi, W.; Abdelhak, J.; Marchivie, M.; Zid, M. F.  
A comparative structural, spectroscopic, optical and photoluminescence studies by DFT of Fe(II) difluoro(oxalato)borate complex  
Journal of Photochemistry and Photobiology a-Chemistry, (352): 43-54. 2018.  
10.1016/j.jphotochem.2017.10.029
- Selvaraj, T.; Rajalingam, R.; Balasubramanian, V.  
Impact of zeolite-Y framework on the geometry and reactivity of Ru (III) benzimidazole complexes - A DFT study  
Applied Surface Science, (434): 781-786. 2018. 10.1016/j.apsusc.2017.11.011
- Semenov, S. G.; Bedrina, M. E.; Titov, A. V.  
A Quantum Chemical Study of C<sub>60</sub>Cl<sub>30</sub>, C-60(OH)(30) Molecules and Fe@C-60(OH)(30) Endocomplex  
Journal of Structural Chemistry, (59): 506-511. 2018. 10.1134/s0022476618030022
- Semenov, V. A.; Samultsev, D. O.; Krivdin, L. B.  
GIAO-DFT calculation of N-15 NMR chemical shifts of Schiff bases: Accuracy factors and protonation effects  
Magnetic Resonance in Chemistry, (56): 727-739. 2018. 10.1002/mrc.4721
- Sen, S.; Patwari, G. N.  
Electrostatics and Dispersion in X-H center dot center dot center dot Y (X = C, N, O; Y = N, O)  
Hydrogen Bonds and Their Role in X-H Vibrational Frequency Shifts

ACS Omega, (3): 18518-18527. 2018. 10.1021/acsomega.8b01802

Septelean, R.; Moraru, I. T.; Kocsor, T. G.; Deak, N.; Saffon-Merceron, N.; Castel, A.; Nemes, G.  
Computational and experimental investigation of phosphaalkenyl germynes from donor-acceptor perspective

Inorganica Chimica Acta, (475): 112-119. 2018. 10.1016/j.ica.2017.08.057

Serdaroglu, G.; Uludag, N.

Concise total synthesis of (+/-)-aspidospermidine and computational study: FT-IR, NMR, NBO, NLO, FMO, MEP diagrams

Journal of Molecular Structure, (1166): 286-303. 2018. 10.1016/j.molstruc.2018.04.050

Sergentu, D. C.; Duignan, T. J.; Autschbach, J.

Ab Initio Study of Covalency in the Ground versus Core-Excited States and X-ray Absorption Spectra of Actinide Complexes

Journal of Physical Chemistry Letters, (9): 5583-5591. 2018. 10.1021/acs.jpclett.8b02412

Sergentu, D. C.; Gendron, F.; Autschbach, J.

Similar ligand-metal bonding for transition metals and actinides? 5f(1) U(C<sub>7</sub>H<sub>7</sub>)(2)(-) versus 3d(n) metallocenes

Chemical Science, (9): 6292-6306. 2018. 10.1039/c7sc05373h

Seridi, L.; Boufelfel, A.

Naringenin encapsulation in beta-CD and in heptakis(2,6-di-O-methyl)-beta-CD:NMR, NBO and QTAIM analysis

Journal of Inclusion Phenomena and Macrocyclic Chemistry, (90): 287-304. 2018.  
10.1007/s10847-018-0785-1

Sert, Y.; Gumus, M.; Gokce, H.; Kani, I.; Koca, I.

Molecular docking, Hirshfeld surface, structural, spectroscopic, electronic, NLO and thermodynamic analyses on novel hybrid compounds containing pyrazole and coumarin cores

Journal of Molecular Structure, (1171): 850-866. 2018. 10.1016/j.molstruc.2018.06.069

Sethio, D.; Oliveira, V.; Kraka, E.

Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy  
Molecules, (23) 2018. 10.3390/molecules23112763

Setiawan, D.; Sethio, D.; Cremer, D.; Kraka, E.

From strong to weak NF bonds: on the design of a new class of fluorinating agents  
Physical Chemistry Chemical Physics, (20): 23913-23927. 2018. 10.1039/c8cp03843k

Sewanthi, S.; Muthu, S.; Raja, M.

Molecular docking, vibrational spectroscopy studies of (RS)-2-(tert-butylamino)-1-(3-chlorophenyl)propan-1-one: A potential adrenaline uptake inhibitor

Journal of Molecular Structure, (1173): 251-260. 2018. 10.1016/j.molstruc.2018.07.001

Seyedkatouli, S.; Vakili, M.; Tayyari, S. F.; Afzali, R.

Molecular structure, spectroscopic studies, and copper-oxygen bond strength of alpha-methyl and alpha-ethyl derivatives of copper (II) acetylacetone; Experimental and theoretical approach

Journal of Molecular Structure, (1160): 107-116. 2018. 10.1016/j.molstruc.2018.01.075

Seyfi, S.; Alizadeh, R.; Ganji, M. D.; Amani, V.

Synthesis, spectral and luminescence study, crystal structure determination and DFT calculation of binuclear palladium(II) complexes

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (190): 298-311. 2018. 10.1016/j.saa.2017.09.024

Shah, T. A.; Alam, U.; Alam, M.; Park, S.; Muneer, M.

Single crystal X-ray structure, spectroscopic and DFT studies of Imidazo 2,1-b thiazole: 2-(3-hydroxy-3-phenylimidazo 2,1-b thiazol-2(3H)-ylidene)-1-phenylethano ne

Journal of Molecular Structure, (1157): 638-653. 2018. 10.1016/j.molstruc.2017.12.074

Shahab, S.; Sheikhi, M.; Filippovich, L.; Dikusar, E.; Yahyaei, H.; Kumar, R.; Khaleghian, M.

Design of geometry, synthesis, spectroscopic (FT-IR, UV/Vis, excited state, polarization) and anisotropy (thermal conductivity and electrical) properties of new synthesized derivatives of (E,E)-azomethines in colored stretched poly (vinyl alcohol) matrix

Journal of Molecular Structure, (1157): 536-550. 2018. 10.1016/j.molstruc.2017.12.094

Shahab, S.; Sheikhi, M.; Filippovich, L.; Khaleghian, M.; Dikusar, E.; Yahyaei, H.; Borzehandani, M. Y.

Spectroscopic Studies (Geometry Optimization, E → Z Isomerization, UV/Vis, Excited States, FT-IR, HOMO-LUMO, FMO, MEP, NBO, Polarization) and Anisotropy of Thermal and Electrical Conductivity of New Azomethine Dyes in Stretched Polymer Matrix

Silicon, (10): 2361-2385. 2018. 10.1007/s12633-018-9773-8

Shahabi, M.; Raissi, H.

Assessment of solvent effects on the inclusion behavior of pyrazinamide drug into cyclic peptide based nanotubes as novel drug delivery vehicles

Journal of Molecular Liquids, (268): 326-334. 2018. 10.1016/j.molliq.2018.07.064

Shahid, M.; Salim, M.; Khalid, M.; Tahir, M. N.; Khan, M. U.; Braga, A. A. C.

Synthetic, XRD, non-covalent interactions and solvent dependent nonlinear optical studies of Sulfadiazine-Ortho-Vanillin Schiff base: (E)-4-((2-hydroxy-3-methoxy-benzylidene) amino)-N-(pyrimidin-2-yl)benzene-sulfonamide

Journal of Molecular Structure, (1161): 66-75. 2018. 10.1016/j.molstruc.2018.02.043

Shajari, N.; Ghiasi, R.

Theoretical Study of Tautomerization in 1,5-Dimethyl-6-Thioxo-1,3,5-Triazinane-2,4-Dione

Journal of Structural Chemistry, (59): 541-549. 2018. 10.1134/s002247661803006x

Shajari, N.; Ghiasi, R.; Ramazani, A.

ONE-POT SYNTHESIS OF 2-ACYLAMINOBENZIMIDAZOLES FROM THE REACTION BETWEEN TRICHLOROACETYL ISOCYANATE AND 1,2-PHENYLENEDIAMINE DERIVATIVES AND THEORETICAL STUDY OF STRUCTURE AND PROPERTIES OF SYNTHESIZED 2-ACYLAMINOBENZIMIDAZOLES

Journal of the Chilean Chemical Society, (63): 3968-3973. 2018. 10.4067/s0717-97072018000203968

Shalabi, A. S.; Aal, S. A.; Soliman, K. A.

Ti functionalized carbon and boron nitride chains: a promising material for hydrogen storage  
Structural Chemistry, (29): 563-576. 2018. 10.1007/s11224-017-1053-5

Shamovsky, I.; Belfield, G.; Lewis, R.; Narjes, F.; Ripa, L.; Tyrchan, C.; Oberg, L.; Sjo, P.

Theoretical studies of the second step of the nitric oxide synthase reaction: Electron tunneling prevents uncoupling

Journal of Inorganic Biochemistry, (181): 28-40. 2018. 10.1016/j.jinorgbio.2018.01.009

Shanmugam, S.; Nachimuthu, S.; Subramaniam, V.

Electronic and optical properties of edge modified peritetracene: a DFT study  
Structural Chemistry, (29): 1853-1865. 2018. 10.1007/s11224-018-1157-6

Shanmugavadivu, T.; Balachandar, S.; Muthuraja, P.; Dhandapani, M.

Structural, computational and Hirshfeld surface analysis of a proton transfer crystal, amino (2-(propan-2-ylidene) hydrazinyl) methaniminium picrate

Journal of Molecular Structure, (1171): 793-807. 2018. 10.1016/j.molstruc.2018.06.021

Sharafie, D.; Amani, V.; Naseh, M.

Synthesis, spectroscopic characterization, crystal structure determination and DFT calculations of Au(Me(2)phen)Br<sub>2</sub> AuBr<sub>2</sub>

Chemical Papers, (72): 1427-1435. 2018. 10.1007/s11696-018-0389-7

Shariatinia, Z.; Abdollahi-Moghadam, M.

DFT computations on surface physical adsorption of hydrocarbons produced in the Fischer-Tropsch synthesis on a CNT/Co nanocatalyst

Journal of Saudi Chemical Society, (22): 786-808. 2018. 10.1016/j.jscs.2018.01.001

Sharma, D.; Sabela, M. I.; Kanchi, S.; Bisetty, K.; Skelton, A. A.; Honarpasvar, B.

Green synthesis, characterization and electrochemical sensing of silymarin by ZnO nanoparticles: Experimental and DFT studies

Journal of Electroanalytical Chemistry, (808): 160-172. 2018. 10.1016/j.jelechem.2017.11.039

Shayan, K.; Nowroozi, A.

Boron nitride nanotubes for delivery of 5-fluorouracil as anticancer drug: a theoretical study  
Applied Surface Science, (428): 500-513. 2018. 10.1016/j.apsusc.2017.09.121

- Sheikhi, M.; Shahab, S.; Filippovich, L.; Yahyaei, H.; Dikusar, E.; Khaleghian, M.  
New derivatives of (E,E)-azomethines: Design, quantum chemical modeling, spectroscopic (FT-IR, UV/Vis, polarization) studies, synthesis and their applications: Experimental and theoretical investigations  
Journal of Molecular Structure, (1152): 368-385. 2018. 10.1016/j.molstruc.2017.09.108
- Shen, C.; Gong, Z. Y.; Gao, L.; Gu, M. L.; Huan, L.; Wang, S. C.; Xie, J.  
Theoretical study on host-guest interaction between pillar 4 arene and molecules or ions  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3736-2
- Shen, S. J.; Zeng, Y. L.; Li, X. Y.; Meng, L. P.; Zhang, X. Y.  
Insight into the -hole center dot center dot center dot-electrons tetrel bonds between F(2)ZO (Z=C, Si, Ge) and unsaturated hydrocarbons  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25521
- Sheng, X. H.; Cui, C. C.; Shan, C.; Li, Y. Z.; Sheng, D. H.; Sun, B.; Chen, D. Z.  
O-Phenylenediamine: a privileged pharmacophore of ferrostatins for radical-trapping reactivity in blocking ferroptosis  
Organic & Biomolecular Chemistry, (16): 3952-3960. 2018. 10.1039/c8ob00546j
- Sherin, D. R.; Manojkumar, T. K.; Rajasekharan, K. N.  
Logic Operations Based on Analyte Response of CRANAD-1: A Simple Molecular Switch Acts as Acid-Base Sensor  
Chemistryselect, (3): 170-175. 2018. 10.1002/slct.201702433
- Shi, R. L.; Wang, P. J.; Tang, L. L.; Huang, X. M.; Chen, Y. G.; Su, Y.; Zhao, J. J.  
Structures and Spectroscopic Properties of F-(H<sub>2</sub>O)(n) with n=1-10 Clusters from a Global Search Based On Density Functional Theory  
Journal of Physical Chemistry A, (122): 3413-3422. 2018. 10.1021/acs.jpca.7b08872
- Shi, Y. L.; Jiang, W. R.; Zhang, Z. Y.; Li, D. H.; Song, H. J.; Wang, Z. G.  
Hydrogen bonding cooperation in glycine-(water)(n) clusters studied by density functional theory calculations  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25556
- Shibata, M.; Ito, H.; Itami, K.  
C-H Arylation of Phenanthrene with Trimethylphenylsilane by Pd/o-Chloranil Catalysis: Computational Studies on the Mechanism, Regioselectivity, and Role of o-Chloranil  
Journal of the American Chemical Society, (140): 2196-2205. 2018. 10.1021/jacs.7b11260
- Shimizu, D.; Fujimoto, K.; Osuka, A.  
Stable Diporphyrinylaminyl Radical and Nitrenium Ion  
Angewandte Chemie-International Edition, (57): 9434-9438. 2018. 10.1002/anie.201805385

Shirai, S.; Sato, S.; Suzuki, T. M.; Jinnouchi, R.; Ohba, N.; Asahi, R.; Morikawa, T.  
Effects of Ta<sub>2</sub>O<sub>5</sub> Surface Modification by NH<sub>3</sub> on the Electronic Structure of a Ru-Complex/N  
Ta<sub>2</sub>O<sub>5</sub> Hybrid Photocatalyst for Selective CO<sub>2</sub> Reduction  
Journal of Physical Chemistry C, (122): 1921-1929. 2018. 10.1021/acs.jpcc.7b09670

Shoaf, A. L.; Bayse, C. A.  
Trigger bond analysis of nitroaromatic energetic materials using wiberg bond indices  
Journal of Computational Chemistry, (39): 1236-1248. 2018. 10.1002/jcc.25186

Shoji, Y.; Shigeno, N.; Takenouchi, K.; Sugimoto, M.; Fukushima, T.  
Mechanistic Study of Highly Efficient Direct 1,2-Carboboration of Alkynes with 9-Borafluorenes  
Chemistry-a European Journal, (24): 13223-13230. 2018. 10.1002/chem.201801818

Shopov, D. Y.; Sharninghausen, L. S.; Sinha, S. B.; Mercado, B. Q.; Balcells, D.; Brudvig, G. W.; Crabtree, R. H.  
A Dinuclear Iridium(V,V) Oxo-Bridged Complex Characterized Using a Bulk Electrolysis Technique  
for Crystallizing Highly Oxidizing Compounds  
Inorganic Chemistry, (57): 5684-5691. 2018. 10.1021/acs.inorgchem.8b00757

Shoyama, K.; Mahl, M.; Seifert, S.; Wurthner, F.  
A General Synthetic Route to Polycyclic Aromatic Dicarboximides by Palladium-Catalyzed  
Annulation Reaction  
Journal of Organic Chemistry, (83): 5339-5346. 2018. 10.1021/acs.joc.8b00301

Shtepliuk, I.; Yakimova, R.  
Interband transitions in closed-shell vacancy containing graphene quantum dots complexed with  
heavy metals  
Physical Chemistry Chemical Physics, (20): 21528-21543. 2018. 10.1039/c8cp03306d

Shukla, M.; Sinha, I.  
Catalytic activation of nitrobenzene on PVP passivated silver cluster: A DFT investigation  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25490

Shukla, R.; Claiser, N.; Souhassou, M.; Lecomte, C.; Balkrishna, S. J.; Kumar, S.; Chopra, D.  
Exploring the simultaneous sigma-hole/pi-hole bonding characteristics of a Br center dot center  
dot center dot pi interaction in an ebselen derivative via experimental and theoretical electron-density  
analysis  
Iucrj, (5): 647-653. 2018. 10.1107/s2052252518011041

Shukla, S.; Bishnoi, A.; Fatma, S.; Verma, A. K.; Devi, P.  
Computational and Experimental FT- IR, NMR, UV-Vis Spectral Studies of 5,5' -((4-  
chlorophenyl)methylene)bis(1,3-dimethyl-6-(methylamino)pyrimidine- 2,4(1H,3H)-dione)  
Chemistryselect, (3): 7800-7808. 2018. 10.1002/slct.201800802

- Sieffert, N.  
Molecular motions in a fluxional ( $\eta(6)$ -indenyl) tricarbonylchromium hemichelate: a density functional theory molecular dynamics study  
*Dalton Transactions*, (47): 8906-8920. 2018. 10.1039/c8dt01779d
- Sifain, A. E.; Lubbers, N.; Nebgen, B. T.; Smith, J. S.; Likhov, A. Y.; Isayev, O.; Roitberg, A. E.; Barros, K.; Tretiak, S.  
Discovering a Transferable Charge Assignment Model Using Machine Learning  
*Journal of Physical Chemistry Letters*, (9): 4495-4501. 2018. 10.1021/acs.jpclett.8b01939
- Sikorska, C.  
Mg<sub>3</sub>F<sub>7</sub>: A superhalogen with potential for new nanomaterials design  
*International Journal of Quantum Chemistry*, (118) 2018. 10.1002/qua.25728
- Silva, P. J.; Bernardo, C. E. P.  
Influence of Alkyne and Azide Substituents on the Choice of the Reaction Mechanism of the Cu+-Catalyzed Addition of Azides to Iodoalkynes  
*Journal of Physical Chemistry A*, (122): 7497-7507. 2018. 10.1021/acs.jpca.8b06894
- Silva, S.; Matsuo, B. T.; da Silva, R. C.; Pozzi, L. V.; Correa, A. G.; Rollin, P.; Zukerman-Schpector, J.; Ferreira, M. A. B.; Paixao, M. W.  
Organocatalyzed Asymmetric Vinyllogous Addition of Oxazole-2(3H)-thiones to alpha,beta-Unsaturated Ketones: An Additive-Free Approach for Diversification of Heterocyclic Scaffold  
*Journal of Organic Chemistry*, (83): 1701-1716. 2018. 10.1021/acs.joc.7b02236
- Silva, S. C.; Rodrigues, S. M. M.; Nardini, V.; Vaz, A. D. L.; Palaretti, V.; da Silva, G. V. J.; Vessecchi, R.; Clososki, G. C.  
Conformational dynamics of 4-formylaminoantipyrine based on NMR and theoretical calculations  
*Journal of Molecular Structure*, (1163): 280-286. 2018. 10.1016/j.molstruc.2018.03.003
- Silveira, R. G.; Catao, A. J. L.; Cunha, B. N.; Almeida, F.; Correa, R. S.; Diniz, L. F.; Tenorio, J. C.; Ellena, J.; Kuznetsov, A. E.; Batista, A. A.; Alcantara, E.  
Facile Synthesis and Characterization of Symmetric N- (Phenylcarbonyl) carbamothioyl benzamide Thiourea: Experimental and Theoretical Investigations  
*Journal of the Brazilian Chemical Society*, (29): 2502-2513. 2018. 10.21577/0103-5053.20180129
- Simon, M.; Milbeo, P.; Liu, H. T.; Andre, C.; Wenger, E.; Martinez, J.; Amblard, M.; Aubert, E.; Legrand, B.; Calmes, M.  
12/10-Helix in Mixed beta-Peptides Alternating Bicyclic and Acyclic beta-Amino Acids: Probing the Relationship between Bicyclic Side Chain and Helix Stability  
*Chemistry-a European Journal*, (24): 18795-18800. 2018. 10.1002/chem.201804404

Simoncic, M.; Urbic, T.

Hydrogen bonding between hydrides of the upper-right part of the periodic table  
Chemical Physics, (507): 34-43. 2018. 10.1016/j.chemphys.2018.03.036

Singh, H.; Singh, S.; Agarwal, P.; Tandon, P.; Erande, R. D.; Dethe, D. H.

Structural and spectroscopic analysis of indole alkaloids: Molecular docking and DFT approach  
Journal of Molecular Structure, (1153): 262-274. 2018. 10.1016/j.molstruc.2017.10.026

Singh, P.; Gupta, A. K.; Sharma, S.; Singh, H. B.; Butcher, R. J.

Synthesis and characterization of N,N ',C-bound organotellurium(IV) and organomercury(II) derivatives

Inorganica Chimica Acta, (483): 218-228. 2018. 10.1016/j.ica.2018.08.016

Singh, P.; Islam, S. S.; Ahmad, H.; Prabaharan, A.

Spectroscopic investigation (FT-IR, FT-Raman), HOMO-LUMO, NBO, and molecular docking analysis of N-ethyl-N-nitrosourea, a potential anticancer agent

Journal of Molecular Structure, (1154): 39-50. 2018. 10.1016/j.molstruc.2017.10.012

Singh, R.; Kaur, P.; Sachdeva, R.; Grewal, J. S.; Sathe, V.; Saini, G. S. S.

Computational study of effect of solvents on vibrational spectra of coumarin 500

Computational and Theoretical Chemistry, (1130): 46-57. 2018. 10.1016/j.comptc.2018.03.008

Singh, R. K.; Iwasa, T.; Taketsugu, T.

Insights into Geometries, Stabilities, Electronic Structures, Reactivity Descriptors, and Magnetic Properties of Bimetallic Ni<sub>m</sub>Cu<sub>n-m</sub> (m=1, 2; n=3-13) Clusters: Comparison with Pure Copper Clusters

Journal of Computational Chemistry, (39): 1878-1889. 2018. 10.1002/jcc.25361

Singh, S. K.; Joshi, P. R.; Shaw, R. A.; Hill, J. G.; Das, A.

Interplay between hydrogen bonding and n- $\pi^*$  interaction in an analgesic drug salicin

Physical Chemistry Chemical Physics, (20): 18361-18373. 2018. 10.1039/c8cp00655e

Siva, W.; Tormena, C. F.; Rittner, R.

Revealing the Conformational Preferences of Proteinogenic Glutamic Acid Derivatives in Solution by <sup>1</sup>H NMR Spectroscopy and Theoretical Calculations

Journal of Physical Chemistry A, (122): 4555-4561. 2018. 10.1021/acs.jpca.8b02523

Sivanadanam, J.; Mukkamala, R.; Mandal, S.; Vedarajan, R.; Matsumi, N.; Aidhen, I. S.; Ramanujam, K.

Exploring the role of the spacers and acceptors on the triphenylamine-based dyes for dye-sensitized solar cells

International Journal of Hydrogen Energy, (43): 4691-4705. 2018.

10.1016/j.ijhydene.2017.10.183

Sivasubramani, V.; George, J.; Pandian, M. S.; Ramasamy, P.; Pounraj, P.; Maurya, K. K.; Sajan, D.

Directional growth, physicochemical and quantum chemical investigations on pyridinium 2-carboxylate: 4-nitrophenol (P2C4N) single crystal for nonlinear optical (NLO) applications  
New Journal of Chemistry, (42): 4261-4277. 2018. 10.1039/c7nj03928j

Skoch, K.; Cisarova, I.; Uhlik, F.; Stepnicka, P.

Comparing the reactivity of isomeric phosphinoferroocene nitrile and isocyanide in Pd(ii) complexes: synthesis of simple coordination compounds vs. preparation of P-chelated insertion products and Fischer-type carbenes

Dalton Transactions, (47): 16082-16101. 2018. 10.1039/c8dt03564d

Slivka, M.; Korol, N.; Fizer, M.; Baumer, V.; Lendel, V.

1,3 Thiazolo 3,2-b 1,2,4 triazol-7-i um salts: synthesis, properties and structural studies  
Heterocyclic Communications, (24): 197-203. 2018. 10.1515/hc-2018-0048

Smirnova, E. S.; Acuna-Pares, F.; Escudero-Adan, E. C.; Jelsch, C.; Lloret-Fillol, J.

Synthesis and Reactivity of Copper(I) Complexes Based on C-3-Symmetric Tripodal HTIM(PR2)(3) Ligands

European Journal of Inorganic Chemistry: 2612-2620. 2018. 10.1002/ejic.201800074

Smith, L. J.; Taimoory, S. M.; Tam, R. Y.; Baker, R. E. G.; Mohammad, N. B.; Trant, J. F.; Shoichet, M. S.

Diels Alder Click-Cross-Linked Hydrogels with Increased Reactivity Enable 3D Cell Encapsulation  
Biomacromolecules, (19): 926-935. 2018. 10.1021/acs.biomac.7b01715

Smitha, M.; Mary, Y. S.; Hossain, M.; Resmi, K. S.; Armakovic, S.; Armakovic, S. J.; Pavithran, R.; Nanda, A. K.; Van Alsenoy, C.

Two novel imidazole derivatives - Combined experimental and computational study  
Journal of Molecular Structure, (1173): 221-239. 2018. 10.1016/j.molstruc.2018.06.110

Smrecki, N.; Kukovec, B. M.; Roncevic, I.; Popovic, Z.

New coordination modes of iminodiacetamide type ligands in palladium(II) complexes:  
crystallographic and DFT studies

Structural Chemistry, (29): 195-206. 2018. 10.1007/s11224-017-1018-8

Sohn, D. H.; Han, E.; Cho, S. J.; Kang, J.

Phosphinate selective hosts and importance of C-H hydrogen bonding for affinity modulation toward anion guests

Tetrahedron Letters, (59): 1728-1732. 2018. 10.1016/j.tetlet.2018.03.066

Soleimani-Amiri, S.; Koohi, M.; Azizi, Z.

Characterization of nonsegregated C<sub>17</sub>Si<sub>3</sub> heterofullerenic isomers using density functional theory method

Journal of the Chinese Chemical Society, (65): 1453-1464. 2018. 10.1002/jccs.201800163

Solel, E.; Kozuch, S.

On the Power of Geometry over Tetrel Bonds  
Molecules, (23) 2018. 10.3390/molecules23112742

Solel, E.; Kozuch, S.

Tuning the Spin, Aromaticity, and Quantum Tunneling in Computationally Designed Fulvalenes  
Journal of Organic Chemistry, (83): 10826-10834. 2018. 10.1021/acs.joc.8b01541

Soleymani, M.

DFT study of double 1,3-dipolar cycloaddition of nitrilimines with allenoates  
Monatshefte fur Chemie, (149): 2183-2193. 2018. 10.1007/s00706-018-2311-y

Soliman, S. M.; Albering, J. H.

Synthesis, X-ray structure and topology (AIM and Hirshfeld) analyses of the new square planar Ag(pyridine-2-aldoxime)(2) ClO<sub>4</sub> complex; A comparative study with its nitro analogue  
Journal of Molecular Structure, (1151): 204-217. 2018. 10.1016/j.molstruc.2017.08.071

Soliman, S. M.; Albering, J. H.; Barakat, A.

Unexpected formation of polymeric silver(I) complexes of azine-type ligand via self-assembly of Ag-salts with isatin oxamohydrazide  
Royal Society Open Science, (5) 2018. 10.1098/rsos.180434;180434

Soliman, S. M.; Barakat, A.; Islam, M. S.; Ghabbour, H. A.

Synthesis, Crystal Structure and DFT Studies of a New Dinuclear Ag(I)-Malonamide Complex  
Molecules, (23) 2018. 10.3390/molecules23040888

Soliman, S. M.; El-Faham, A.

Low temperature X-ray structure analyses combined with NBO studies of a new heteroleptic octa-coordinated Holmium(III) complex with N,N,N-tridentate hydrazono-phthalazine-type ligand  
Journal of Molecular Structure, (1157): 222-229. 2018. 10.1016/j.molstruc.2017.12.016

Soliman, S. M.; El-Faham, A.

One pot synthesis of two Mn(II) perchlorate complexes with s-triazine NNN-pincer ligand; molecular structure, Hirshfeld analysis and DFT studies  
Journal of Molecular Structure, (1164): 344-353. 2018. 10.1016/j.molstruc.2018.03.037

Soliman, S. M.; El-Faham, A.

Synthesis, characterization, and structural studies of two heteroleptic Mn(II) complexes with tridentate N,N,N-pincer type ligand  
Journal of Coordination Chemistry, (71): 2373-2388. 2018. 10.1080/00958972.2018.1475660

Soliman, S. M.; El-Faham, A.; Elsilk, S. E.; Farooq, M.

Two heptacoordinated manganese(II) complexes of giant pentadentate s-triazine bis-Schiff base ligand: Synthesis, crystal structure, biological and DFT studies  
Inorganica Chimica Acta, (479): 275-285. 2018. 10.1016/j.ica.2018.04.043

Soliman, S. M.; Elsilk, S. E.

Synthesis, X-ray structure, DFT and antimicrobial studies of Ag(I) complexes with nicotinic acid derivatives

Journal of Photochemistry and Photobiology B-Biology, (187): 48-53. 2018.

10.1016/j.jphotobiol.2018.07.029

Solimannejad, M.; Kamalinahad, S.; Shakerzadeh, E.

Silicon carbide nanotubes (SiCNTs) serving for catalytic decomposition of toxic diazomethane (DAZM) gas: a DFT study

Molecular Physics, (116): 414-422. 2018. 10.1080/00268976.2017.1396370

Solimannejad, M.; Rezaie, F.; Kamalinahad, S.

Correlating cluster size and NLO response of complexes aggregated with bifurcated metal bonds: a DFT study

Structural Chemistry, (29): 119-127. 2018. 10.1007/s11224-017-1009-9

Soltani, A.; Javan, M. B.; Raz, S. G.; Mashkoor, R.; Khalaji, A. D.; Dusek, M.; Fejfarova, K.; Palatinus, L.; Rohlicek, J.; Machek, P.

Crystallography, vibrational, electronic and optical analysis of 4-Bromo-2-(2,5-dichlorophenylimino)-phenol

Journal of Molecular Structure, (1173): 521-530. 2018. 10.1016/j.molstruc.2018.01.009

Song, J. J.; Su, Y.; Jia, Y. P.; Chen, L. S.; Zhang, G. Q.

Resonance bonding in XNgY (X = F, Cl, Br, I; Ng = Kr or Xe; Y = CN or NC) molecules: an NBO/NRT investigation

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3665-0

Song, M. J.; Yang, F.; Liu, L.; Shen, L. P.; Hu, P. F.; Su, C. X.

Experimental and theoretical study of fingerprint spectra of 2-(4-fluorophenyl)benzimidazole and 2-(4-chlorophenyl)benzimidazole in terahertz range

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (202): 18-29. 2018.

10.1016/j.saa.2018.04.077

Song, Y. L.; Lu, X. F.; Sheng, Y.; Geng, Z. Y.

Theoretical investigation of auxiliary electronic acceptors in modifying D-D--A sensitizers for dye-sensitized solar cells

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3871-9

Song, Y. L.; Lu, X. F.; Sheng, Y.; Zhao, G. R.; Wang, G. Y.; Geng, Z. Y.

Theoretical investigations on newly designed triphenylamine- based donors applied into the D-pi-A and D-A-pi-A type sensitizers

Journal of Computational Electronics, (17): 1816-1834. 2018. 10.1007/s10825-018-1246-1

Sonmez, M.; Nazir, H.; Emir, E.; Svoboda, I.; Aksu, L.; Atakol, O.  
Two dinuclear Ni-II-Cd-II complexes of reduced ONNO-type Schiff bases  
Journal of Thermal Analysis and Calorimetry, (131): 3077-3091. 2018. 10.1007/s10973-017-6720-7

Sorbelli, D.; Belpassi, L.; Tarantelli, F.; Belanzoni, P.  
Ligand Effect on Bonding in Gold(III) Carbonyl Complexes  
Inorganic Chemistry, (57): 6161-6175. 2018. 10.1021/acsinorgchem.8b00765

Spinello, A.; Pavlin, M.; Casalino, L.; Magistrato, A.  
A Dehydrogenase Dual Hydrogen Abstraction Mechanism Promotes Estrogen Biosynthesis: Can We Expand the Functional Annotation of the Aromatase Enzyme?  
Chemistry-a European Journal, (24): 10840-10849. 2018. 10.1002/chem.201802025

Sproviero, E. M.  
Intramolecular Natural Energy Decomposition Analysis: Applications to the Rational Design of Foldamers  
Journal of Computational Chemistry, (39): 1367-1386. 2018. 10.1002/jcc.25127

Sreelaja, P. V.; Ravikumar, C.  
Scaled Quantum Chemical Studies and Vibrational Spectra of Conjugated Structure 2-Benzylidenehydrazinecarbothioamide  
Optics and Spectroscopy, (125): 609-618. 2018. 10.1134/s0030400x18110292

Sreenath, M. C.; Joe, I. H.; Rastogi, V. K.  
Experimental and theoretical investigation of third-order nonlinear optical properties of azo dye 1-(2, 5-Dimethoxy-phenylazo)-naphthalen-2-ol by Z-scan technique and quantum chemical computations  
Dyes and Pigments, (157): 163-178. 2018. 10.1016/j.dyepig.2018.04.044

Sreenath, M. C.; Joe, I. H.; Rastogi, V. K.  
Third-order optical nonlinearities of 1,5-Diaminoanthraquinone for optical limiting application  
Optics and Laser Technology, (108): 218-234. 2018. 10.1016/j.optlastec.2018.06.056

Srivastava, A. K.  
Reduction of nitrogen oxides (NO<sub>x</sub>) by superalkalis  
Chemical Physics Letters, (695): 205-210. 2018. 10.1016/j.cplett.2018.02.029

Srivastava, A. K.; Pandey, S. K.; Pandey, A. K.; Misra, N.  
C-60 as Electron Acceptor and Donor: A Comparative DFT Study of Li@C-60 and F@C-60  
Australian Journal of Chemistry, (71): 953-956. 2018. 10.1071/ch18391

Srivastava, D. J.; Florian, P.; Baltisberger, J. H.; Grandinetti, P. J.  
Correlating geminal (2J)Si-O-Si) couplings to structure in framework silicates

Physical Chemistry Chemical Physics, (20): 562-571. 2018. 10.1039/c7cp06486a

Srivastava, K.; Khan, E.; Shimpi, M. R.; Tandon, P.; Sinha, K.; Velaga, S. P.

Molecular structure and hydrogen bond interactions of a paracetamol-4,4'-bipyridine cocrystal studied using a vibrational spectroscopic and quantum chemical approach

Crystengcomm, (20): 213-222. 2018. 10.1039/c7ce01505d

Srivastava, R.

Theoretical studies on the electronic and optoelectronic properties of A.2

AP(w)/A\*.2AP(WC)/C.2AP(w)/C\*.2AP(WC)/C.A(w)/C\*.A(WC) -Au-8 mismatch nucleobase complexes

Molecular Physics, (116): 263-272. 2018. 10.1080/00268976.2017.1382737

Sruthi, P. K.; Ramanathan, N.; Sarkar, S.; Sundararajan, K.

Pentavalent phosphorus as a unique phosphorus donor in POCl<sub>3</sub> homodimer and POCl<sub>3</sub>-H<sub>2</sub>O heterodimer: matrix isolation infrared spectroscopic and computational studies

Physical Chemistry Chemical Physics, (20): 22058-22075. 2018. 10.1039/c8cp03937b

Stasyuk, A. J.; Sola, M.; Voityuk, A. A.

Reliable charge assessment on encapsulated fragment for endohedral systems

Scientific Reports, (8) 2018. 10.1038/s41598-018-21240-0

Steglich, M.; Bodí, A.; Maier, J. P.; Hemberger, P.

Probing different spin states in xylyl radicals and ions

Physical Chemistry Chemical Physics, (20): 7180-7189. 2018. 10.1039/c7cp08466h

Stellato, F.; Calandra, M.; D'Acapito, F.; De Santis, E.; La Penna, G.; Rossi, G.; Morante, S.

Multi-scale theoretical approach to X-ray absorption spectra in disordered systems: an application to the study of Zn(II) in water

Physical Chemistry Chemical Physics, (20): 24775-24782. 2018. 10.1039/c8cp04355h

Stojanovic, M.; Baranac-Stojanovic, M.

Analysis of Stability and (Anti)aromaticity of BN-Dibenzo a, e pentalenes

European Journal of Organic Chemistry: 6230-6240. 2018. 10.1002/ejoc.201801047

Stojanovic, M.; Baranac-Stojanovic, M.

Mono BN-substituted analogues of naphthalene: a theoretical analysis of the effect of BN position on stability, aromaticity and frontier orbital energies

New Journal of Chemistry, (42): 12968-12976. 2018. 10.1039/c8nj01529e

Stone, A. J.; Szalewicz, K.

Reply to "Comment on 'Natural Bond Orbitals and the Nature of the Hydrogen Bond'"

Journal of Physical Chemistry A, (122): 733-736. 2018. 10.1021/acs.jpca.7b09307

Su, Z. S.; Zuo, Y. N.; Hu, C. W.

Theoretical Investigation on Direct Vinylogous Aldol Reaction of Isatin Catalyzed by Chiral-N, N'-dioxide Sc(III) Complex

Molecular Catalysis, (453): 22-30. 2018. 10.1016/j.mcat.2018.04.025

Subhapriya, G.; Kalyanaraman, S.; Jeyachandran, M.; Ragavendran, V.; Krishnakumar, V.

Experimental and theoretical studies on the structural, spectroscopic and hydrogen bonding on 4-nitro-n-(2,4-dinitrophenyl) benzenamine

Journal of Molecular Structure, (1158): 139-144. 2018. 10.1016/j.molstruc.2018.01.019

Subhasri, P.; Jayaprakasam, R.; Vijayakumar, V. N.

Experimental and computational (DFT) studies on induced orthogonal smectic A\* phase in hydrogen-bonded ferroelectric liquid crystals

International Journal of Modern Physics B, (32) 2018. 10.1142/s0217979218502235

Subhasri, P.; Venugopal, D.; Jayaprakasam, R.; Chitravel, T.; Vijayakumar, V. N.

Observation of paramorphic phenomenon and non-tilted orthogonal smectic phases in hydrogen bonded ferroelectric liquid crystals for photonic applications

Physica B-Condensed Matter, (539): 78-87. 2018. 10.1016/j.physb.2018.04.001

Suenaga, M.; Nakata, K.; Abboud, J. L. M.; Mishima, M.

A natural bond orbital analysis of aryl-substituted polyfluorinated carbanions: negative hyperconjugation

Journal of Physical Organic Chemistry, (31) 2018. 10.1002/poc.3721

Sugahara, T.; Sasamori, T.; Tokitoh, N.

2,5-Digermaselenophenes: Germanium Analogues of Selenophenes

Journal of the American Chemical Society, (140): 11206-11209. 2018. 10.1021/jacs.8b07588

Sugahara, T.; Sasamori, T.; Tokitoh, N.

Chalcogenation Reaction of Cyclic Digermenanes

Chemistry Letters, (47): 719-722. 2018. 10.1246/cl.180188

Sugamata, K.; Hashizume, D.; Suzuki, Y.; Sasamori, T.; Ishii, S.

Synthesis and Structure of a Stable Bis(methylene)-lambda(4)-sulfane

Chemistry-a European Journal, (24): 6922-6926. 2018. 10.1002/chem.201800828

Sumii, Y.; Sugita, Y.; Tokunaga, E.; Shibata, N.

Synthesis of Aryl Triflones through the Trifluoromethanesulfonylation of Benzyne

Chemistryopen, (7): 204-211. 2018. 10.1002/open.201700204

Sumrra, S. H.; Atif, A. H.; Zafar, M. N.; Khalid, M.; Tahir, M. N.; Nazar, M. F.; Nadeem, M. A.; Braga, A. A. C.

Synthesis, crystal structure, spectral and DFT studies of potent isatin derived metal complexes

Journal of Molecular Structure, (1166): 110-120. 2018. 10.1016/j.molstruc.2018.03.132

Sumrra, S. H.; Kausar, S.; Raza, M. A.; Zubair, M.; Zafar, M. N.; Nadeem, M. A.; Mughal, E. U.; Chohan, Z. H.; Mushtaq, F.; Rashid, U.

Metal based triazole compounds: Their synthesis, computational, antioxidant, enzyme inhibition and antimicrobial properties

Journal of Molecular Structure, (1168): 202-211. 2018. 10.1016/j.molstruc.2018.05.036

Sun, C. F.; Zhao, H. F.; Liu, X. C.; Yin, H.; Shi, Y.

Tunable ESIPT reaction and antioxidant activities of 3-hydroxyflavone and its derivatives by altering atomic electronegativity

Organic Chemistry Frontiers, (5): 3435-3442. 2018. 10.1039/c8qo00998h

Sun, H. Q.; Zhang, W. J.; Xu, N.

Density functional calculation of structural and electronic properties of Ti & IT; $n$  & IT;-& IT; $x$  & IT; Al & IT; $(x)$ & IT; (& IT; $n$  & IT; $=2-8, 13$ , & IT; $x$  & IT; $=0$ -& IT; $n$  & IT;) clusters

Journal of Physics and Chemistry of Solids, (118): 126-136. 2018. 10.1016/j.jpcs.2018.01.029

Sun, P. L.; Rao, D. L.; Zhang, P.; Qin, Y. J.; Guo, Z. X.

Protonation behaviour of 2-phenyl-1,3-diazaazulene derivatives

Tetrahedron, (74): 731-739. 2018. 10.1016/j.tet.2017.12.051

Sun, Q. M.; Berkelbach, T. C.; Blunt, N. S.; Booth, G. H.; Guo, S.; Li, Z. D.; Liu, J. Z.; McClain, J. D.; Sayfutyarova, E. R.; Sharma, S.; Wouters, S.; Chan, G. K. L.

PYSCF: the Python-based simulations of chemistry framework

Wiley Interdisciplinary Reviews-Computational Molecular Science, (8) 2018. 10.1002/wcms.1340

Sun, T. T.; Xie, Q.; Zhao, L.; Zhu, J.

Probing the Most Aromatic and Antiaromatic Pyrrolium Rings by Maximizing Hyperconjugation and Push-Pull Effect

Chemistry-an Asian Journal, (13): 1419-1423. 2018. 10.1002/asia.201800179

Sun, W. H.; Lozada, I. B.; van Wijngaarden, J.

Fourier Transform Microwave Spectroscopic and ab Initio Study of the Rotamers of 2-Fluorobenzaldehyde and 3-Fluorobenzaldehyde

Journal of Physical Chemistry A, (122): 2060-2068. 2018. 10.1021/acs.jpca.7b11673

Sun, W. M.; Wu, D.; Kang, J.; Li, C. Y.; Chen, J. H.; Li, Y.; Li, Z. R.

Decorating Zintl polyanions with alkali metal cations: A novel strategy to design superatom cations with low electron affinity

Journal of Alloys and Compounds, (740): 400-405. 2018. 10.1016/j.jallcom.2017.12.075

Sun, Y. H.; Sun, X. L.; Huang, X. R.

Reaction of CO<sub>2</sub> with Atomic Transition Metal M+/0/- Ions: A Theoretical Study

Journal of Physical Chemistry A, (122): 5848-5860. 2018. 10.1021/acs.jpca.8b01917

Sun, Z.; Moore, K. B.; Hill, J. G.; Peterson, K. A.; Schaefer, H. F.; Hoffmann, R.

Alkali-Metal Trihalides: M+X<sub>3</sub>- Ion Pair or MX-X-2 Complex?

Journal of Physical Chemistry B, (122): 3339-3353. 2018. 10.1021/acs.jpcb.7b10005

Sureshkumar, B.; Mary, Y. S.; Resmi, K. S.; Panicker, C. Y.; Armakovic, S.; Armakovic, S. J.; Van Alsenoy, C.; Narayana, B.; Suma, S.

Spectroscopic analysis of 8-hydroxyquinoline derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations

Journal of Molecular Structure, (1156): 336-347. 2018. 10.1016/j.molstruc.2017.11.120

Sureshkumar, B.; Mary, Y. S.; Resmi, K. S.; Sumo, S.; Armakovic, S.; Armakovic, S. J.; Van Alsenoy, C.; Narayana, B.; Sobhana, D.

Spectroscopic characterization of hydroxyquinoline derivatives with bromine and iodine atoms and theoretical investigation by DFT calculations, MD simulations and molecular docking studies

Journal of Molecular Structure, (1167): 95-106. 2018. 10.1016/j.molstruc.2018.04.077

Sureshkumar, B.; Mary, Y. S.; Suma, S.; Armakovic, S.; Armakovic, S. J.; Van Alsenoy, C.; Narayana, B.; Sasidharan, B. P.

Spectroscopic characterization of 8-hydroxy-5-nitroquinoline and 5-chloro-8-hydroxy quinoline and investigation of its reactive properties by DFT calculations and molecular dynamics simulations

Journal of Molecular Structure, (1164): 525-538. 2018. 10.1016/j.molstruc.2018.03.088

Sutradhar, D.; Bhattacharai, S.; Zeegers-Huyskens, T.; Chandra, A. K.

Unusual Fluorine Substitution Effect on S center dot center dot center dot Cl Bonding between Sulfides and Atomic Chlorine

Journal of Physical Chemistry A, (122): 7142-7150. 2018. 10.1021/acs.jpca.8b04495

Sutradhar, D.; Chandra, A. K.

Halogen bonding between substituted chlorobenzene and trimethylamine: Decisive role of sigma-hole and CCl bond breaking energy

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25511

Suzuki, K.; Numata, Y.; Fujita, N.; Hayakawa, N.; Tanikawa, T.; Hashizume, D.; Tamao, K.; Fueno, H.; Tanaka, K.; Matsuo, T.

A stable free tetragermacyclobutadiene incorporating fused-ring bulky EMind groups

Chemical Communications, (54) 2018. 10.1039/c7cc09443d

Suzuki, Y.; Iwata, N.; Dobashi, K.; Takashima, R.; Arulmozhiraja, S.; Ishitsubo, E.; Matsuo, N.; Tokiwa, H.

Alkanoylation of quinazoline by nucleophilic aromatic substitution: Combined experimental and computational study

Tetrahedron, (74): 392-400. 2018. 10.1016/j.tet.2017.11.071

Suzuki, Y.; Sasamori, T.; Guo, J. D.; Tokitoh, N.

A Redox-Active Bis(ferrocenyl)germylene and Its Reactivity  
Chemistry-a European Journal, (24): 364-368. 2018. 10.1002/chem.201705598

Swiderek, K.; Nodling, A. R.; Tsai, Y. H.; Luk, L. Y. P.; Moliner, V.  
Reaction Mechanism of Organocatalytic Michael Addition of Nitromethane to Cinnamaldehyde:  
A Case Study on Catalyst Regeneration and Solvent Effects  
Journal of Physical Chemistry A, (122): 451-459. 2018. 10.1021/acs.jpca.7b11803

Szczepanik, D. W.  
A simple alternative to the pseudo- method  
International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25696

Szell, P. M. J.; Cavallo, G.; Terraneo, G.; Metrangolo, P.; Gabidullin, B.; Bryce, D. L.  
Comparing the Halogen Bond to the Hydrogen Bond by Solid-State NMR Spectroscopy: Anion  
Coordinated Dimers from 2-and 3-Iodoethynylpyridine Salts  
Chemistry-a European Journal, (24): 11364-11376. 2018. 10.1002/chem.201801279

Szkop, K. M.; Jupp, A. R.; Stephan, D. W.  
P,P-Dimethylformylphosphine: The Phosphorus Analogue of N,N-Dimethylformamide  
Journal of the American Chemical Society, (140): 12751-12755. 2018. 10.1021/jacs.8b09266

Szterner, P.; Amaral, L.; Morais, V. M. F.; da Silva, M.; da Silva, M.  
Energetic characterization of a bioactive compound: Uridine  
Journal of Chemical Thermodynamics, (124): 90-97. 2018. 10.1016/j.jct.2018.04.013

Tabtimsai, C.; Ruangpornvisuti, V.; Tontapha, S.; Wanno, B.  
A DFT investigation on group 8B transition metal-doped silicon carbide nanotubes for hydrogen  
storage application  
Applied Surface Science, (439): 494-505. 2018. 10.1016/j.apsusc.2017.12.255

Tabtimsai, C.; Somtua, T.; Motongsri, T.; Wanno, B.  
A DFT study of H<sub>2</sub>CO and HCN adsorptions on 3d, 4d, and 5d transition metal-doped graphene  
nanosheets  
Structural Chemistry, (29): 147-157. 2018. 10.1007/s11224-017-1013-0

Tahchieva, D. N.; Bakowies, D.; Ramakrishnan, R.; von Lilienfeld, O. A.  
Torsional Potentials of Glyoxal, Oxalyl Halides, and Their Thiocarbonyl Derivatives: Challenges  
for Popular Density Functional Approximations  
Journal of Chemical Theory and Computation, (14): 4806-4817. 2018. 10.1021/acs.jctc.8b00174

Taherpour, A.; Jamshidi, M.; Rezaei, O.; Belverdi, A. R.  
Photoinduced electron transfer process on emission spectrum of N,N'-bis(salicylidene)-1,2-  
phenylenediamine as a Mg<sup>2+</sup> cation chemosensor: A first principle DFT and TDDFT study  
Journal of Molecular Structure, (1161): 339-344. 2018. 10.1016/j.molstruc.2018.02.064

Taherpour, A.; Shahri, Z.; Rezaei, O.; Jamshidi, M.; Fellowes, T.  
Adsorption, intercalation and sensing of helium on yttrium functionalized open edge boron nitride: A first principle DFT and TDDFT study  
Chemical Physics Letters, (691): 231-237. 2018. 10.1016/j.cplett.2017.11.033

Tahtinen, P.; Guella, G.; Saielli, G.; Debitus, C.; Hnawia, E.; Mancini, I.  
New Sulfur-Containing Polyarsenicals from the New Caledonian Sponge Echinocalina bargibanti  
Marine Drugs, (16) 2018. 10.3390/md16100382

Takaki, D.; Ogata, K.; Kurihara, Y.; Ueda, K.; Hashimoto, T.; Yamaguchi, Y.  
Synthesis and reactivity of M(eta(3)-allyl)(eta(2)-amidinato) (CO)(2)(phosphonium ylide) (M = Mo, W): Investigation of the ligand properties of phosphonium ylides  
Inorganica Chimica Acta, (471): 310-315. 2018. 10.1016/j.ica.2017.11.019

Takemoto, S.; Tsujimoto, T.; Matsuzaka, H.  
Anionic Trinuclear Iridium(I) Oxo Complex: Synthesis and Reactivity as a Metal-Centered sigma-Donor Ligand to Gold(I) and Silver(I)  
Organometallics, (37): 1591-1597. 2018. 10.1021/acs.organomet.8b00159

Takjoo, R.; Centore, R.; Hayatolgheibi, S. S.  
Mixed ligand complexes of cadmium(II) and copper(II) dithiocarbazate: Synthesis, spectral characterization, X-ray crystal structure  
Inorganica Chimica Acta, (471): 587-594. 2018. 10.1016/j.ica.2017.11.043

Tamer, O.; Avci, D.; Celikoglu, E.; Idil, O.; Atalay, Y.  
Crystal growth, structural and spectroscopic characterization, antimicrobial activity, DNA cleavage, molecular docking and density functional theory calculations of Zn(II) complex with 2-pyridinecarboxylic acid  
Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4540

Tan, Z.; Li, A. Y.  
Noble gas supported boron-pentagonal clusters B(5)Ng(n)(3+): exploring the structures and bonding  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3605-z

Tanaka, M.; Nakagawa, A.; Nishi, N.; Iijima, K.; Sawa, R.; Takahashi, D.; Toshima, K.  
Boronic-Acid-Catalyzed Regioselective and 1,2-cis-Stereoselective Glycosylation of Unprotected Sugar Acceptors via S(N)i-Type Mechanism  
Journal of the American Chemical Society, (140): 3644-3651. 2018. 10.1021/jacs.7b12108

Tanaka, S.; Nakashima, T.; Maeda, T.; Ratanasak, M.; Hasegawa, J. Y.; Kon, Y.; Tamura, M.; Sato, K.  
Quaternary Alkyl Ammonium Salt-Catalyzed Transformation of Glycidol to Glycidyl Esters by Transesterification of Methyl Esters

ACS Catalysis, (8): 1097-1103. 2018. 10.1021/acscatal.7b03303

Tandaric, T.; Vianello, R.

Design of Exceptionally Strong Organic Superbases Based on Aromatic Pnictogen Oxides: Computational DFT Analysis of the Oxygen Basicity in the Gas Phase and Acetonitrile Solution  
Journal of Physical Chemistry A, (122): 1464-1471. 2018. 10.1021/acs.jpca.7b11945

Tang, H. F.; Zhong, H.; Zhang, L. L.; Gong, M. X.; Song, S. Q.; Tian, Q. P.

Theoretical investigations into the intermolecular hydrogen-bonding interactions of N-(hydroxymethyl)acetamide dimers

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3672-1

Tang, J. Y.; Shen, J. S.; Chen, L.; Jiang, J. W.; Lu, J.; Zhao, X.; Dai, G. L.

Investigation of carbon monoxide catalytic oxidation on vanadium-embedded graphene  
Monatshefte fur Chemie, (149): 1349-1356. 2018. 10.1007/s00706-018-2181-3

Tang, S. S.; Tsона, N. T.; Du, L.

Ring-Size Effects on the Stability and Spectral Shifts of Hydrogen Bonded Cyclic Ethers Complexes

Scientific Reports, (8) 2018. 10.1038/s41598-017-18191-3

Tang, Z.; Yang, Y. F.; Yang, Y.; Wang, Y.; Tian, J.; Fei, X.

Theoretical investigation of twisted charge-transfer-promoted intramolecular proton transfer in the excited state of 4'-dimethylaminoflavonol in a highly polar solvent

Journal of Luminescence, (194): 785-790. 2018. 10.1016/j.jlumin.2017.09.051

Tanimoto, R.; Yamada, K.; Suzuki, S.; Kozaki, M.; Okada, K.

Group 11 Metal Complexes Coordinated by the (Nitronyl Nitroxide)-2-ide Radical Anion: Facile Oxidation of Stable Radicals Controlled by Metal-Carbon Bonds in Radical-Metalloids

European Journal of Inorganic Chemistry: 1198-1203. 2018. 10.1002/ejic.201800038

Tankov, I.; Yankova, R.

Theoretical (density functional theory) studies on the structural, electronic and catalytic properties of the ionic liquid 4-amino-1H-1,2,4-triazolium nitrate

Journal of Molecular Liquids, (269): 529-539. 2018. 10.1016/j.molliq.2018.08.041

Tao, Y. W.; Tian, C.; Verma, N.; Zou, W. L.; Wang, C.; Cremer, D.; Kraka, E.

Recovering Intrinsic Fragmental Vibrations Using the Generalized Subsystem Vibrational Analysis  
Journal of Chemical Theory and Computation, (14): 2558-2569. 2018. 10.1021/acs.jctc.7b01171

Tarahhom, A.; Van Der Lee, A.

A new six-coordinate organotin(IV) complex of OP NC<sub>5</sub>H<sub>10</sub> (3): A comparison with an analogous five-coordinate complex by means of X-ray crystallography, Hirshfeld surface analysis and DFT calculations

Journal of Coordination Chemistry, (71): 1575-1592. 2018. 10.1080/00958972.2018.1461847

Tavanei, L.; Nori-Shargh, D.

New Insights into the Origin of the cis-Configuration Preferences in 1,2-Dihaloethenes: The Importance of the Bonding Orbital Deviations

Australian Journal of Chemistry, (71): 1-13. 2018. 10.1071/ch17219

Taylor, W. S.; Pedder, R. E.; Eden, A. B.; Emmerling, C. L.

Systematic Ligand Effects in the Reactions of Fe+(D-6) and FeX+((5)Delta) with CF<sub>3</sub>X (X = Cl, Br, I). Ion Mobility Measurements of FeX+((5)Delta) (X = F, Cl, Br, I) in He

Journal of Physical Chemistry A, (122): 6509-6523. 2018. 10.1021/acs.jpca.8b05708

Techikawara, K.; Kobayashi, H.; Fukuoka, A.

Conversion of N-Acetylglucosamine to Protected Amino Acid over Ru/C Catalyst

ACS Sustainable Chemistry & Engineering, (6): 12411-12418. 2018.

10.1021/acssuschemeng.8b02951

Teixeira, F.; Melo, A.; Cordeiro, M.

Exploring rare chemical phenomena using fractional nuclear charges: The cis-effect in N<sub>2</sub>F<sub>2</sub>

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25662

Teran, J. E.; Zambrano, C. H.; Mora, J. R.; Rincon, L.; Torres, F. J.

Theoretical investigation of the mechanism for the reductive dehalogenation of methyl halides mediated by the Co-I-based compounds cobalamin and cobaloxime

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3844-z

Terencio, T.; Roithova, J.; Brandes, S.; Rousselin, Y.; Penouilh, M. J.; Meyer, M.

A Comparative IRMPD and DFT Study of Fe<sup>3+</sup> and UO<sub>2</sub><sup>2+</sup> Complexation with N-Methylacetohydroxamic Acid

Inorganic Chemistry, (57): 1125-1135. 2018. 10.1021/acs.inorgchem.7b02567

Testa, A.; Lucas, X.; Castro, G. V.; Chan, K. H.; Wright, J. E.; Runcie, A. C.; Gadd, M. S.; Harrison, W. T. A.; Ko, E. J.; Fletcher, D.; Ciulli, A.

3-Fluoro-4-hydroxyprolines: Synthesis, Conformational Analysis, and Stereoselective Recognition by the VHL E3 Ubiquitin Ligase for Targeted Protein Degradation

Journal of the American Chemical Society, (140): 9299-9313. 2018. 10.1021/jacs.8b05807

Tetteh, S.

Coordination Behavior of Ni<sup>2+</sup>, Cu<sup>2+</sup>, and Zn<sup>2+</sup> in Tetrahedral 1-Methylimidazole Complexes: A DFT/CSD Study

Bioinorganic Chemistry and Applications, 2018. 10.1155/2018/3157969

Tetteh, S.; Zugle, R.; Adotey, J. P. K.; Quashie, A.

Electronic Spectra of ortho-Substituted Phenols: An Experimental and DFT Study

Journal of Spectroscopy, 2018. 10.1155/2018/4193657

Thacker, J. C. R.; Popelier, P. L. A.

Fluorine Gauche Effect Explained by Electrostatic Polarization Instead of Hyperconjugation: An Interacting Quantum Atoms (IQA) and Relative Energy Gradient (REG) Study

Journal of Physical Chemistry A, (122): 1439-1450. 2018. 10.1021/acs.jpca.7b11881

Thacker, J. C. R.; Vincent, M. A.; Popelier, P. L. A.

Using the Relative Energy Gradient Method with Interacting Quantum Atoms to Determine the Reaction Mechanism and Catalytic Effects in the Peptide Hydrolysis in HIV-1 Protease

Chemistry-a European Journal, (24): 11200-11210. 2018. 10.1002/chem.201802035

Thangavel, S.; Paulpandi, M.; Friedrich, H. B.; Sukesh, K.; Skelton, A. A.

New Ru(II) half sandwich complexes bearing the N,N' bidentate 9-ethyl-N-(pyridin-2-ylmethylene)9H-carbazole-3-amine ligand: Effects of halogen (Cl-, Br- and I-) leaving groups versus in vitro activity on HepG2 cancer cells, cell cycle, fluorescence study, cellular accumulation and DFT study

Polyhedron, (152): 37-48. 2018. 10.1016/j.poly.2018.05.060

Thirman, J.; Engelage, E.; Huber, S. M.; Head-Gordon, M.

Characterizing the interplay of Pauli repulsion, electrostatics, dispersion and charge transfer in halogen bonding with energy decomposition analysis

Physical Chemistry Chemical Physics, (20): 905-915. 2018. 10.1039/c7cp06959f

Thirunavukkarasu, K.; Rajkumar, P.; Selvaraj, S.; Suganya, R.; Kesavan, M.; Gunasekaran, S.; Kumaresan, S.

Vibrational (FT-IR and FT-Raman), electronic (UV-Vis), NMR (H-1 and C-13) spectra and molecular docking analyses of anticancer molecule 4-hydroxy-3-methoxycinnamaldehyde

Journal of Molecular Structure, (1173): 307-320. 2018. 10.1016/j.molstruc.2018.07.003

Thomas, C. M.; Hatzis, G. P.; Pepi, M. J.

Examining the effects of variations in ligand framework and pnictogen substitution on the geometry and electronic structure of metal complexes of N-heterocyclic phosphido ligands incorporated into a diphosphine pincer ligand framework

Polyhedron, (143): 215-222. 2018. 10.1016/j.poly.2017.11.015

Thomas, R.; Hossain, M.; Mary, Y. S.; Resmi, K. S.; Armakovic, S.; Armakovic, S. J.; Nanda, A. K.; Ranjan, V. K.; Vijayakumar, G.; Van Alsenoy, C.

Spectroscopic analysis and molecular docking of imidazole derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations

Journal of Molecular Structure, (1158): 156-175. 2018. 10.1016/j.molstruc.2018.01.021

Thompson, M. C.; Weber, J. M.

Infrared Photodissociation Spectra of Sn(CO<sub>2</sub>)(n) (-) Cluster Ions

Journal of Physical Chemistry A, (122): 3772-3779. 2018. 10.1021/acs.jpca.8b00362

- Thomsen, M. K.; Gatti, C.; Overgaard, J.  
Probing Cyclic pi-Electron Delocalization in an Imidazol-2-ylidene and a Corresponding Imidazolium Salt  
Chemistry-a European Journal, (24): 4973-4981. 2018. 10.1002/chem.201800014
- Thongnuam, W.; Maihom, T.; Choomwattana, S.; Injongkol, Y.; Boekfa, B.; Treesukol, P.; Limtrakul, J.  
Theoretical study of CO<sub>2</sub> hydrogenation into formic acid on Lewis acid zeolites  
Physical Chemistry Chemical Physics, (20): 25179-25185. 2018. 10.1039/c8cp03146k
- Thorley, K. J.; McCulloch, I.  
Why are S-F and S-O non-covalent interactions stabilising?  
Journal of Materials Chemistry C, (6): 12413-12421. 2018. 10.1039/c8tc04252g
- Thottiparambil, A.; Purushothaman, I.; De, S.; Parameswaran, P.; Beegum, P. S.; Antharjanam, P. K. S.; Chakkumkumarath, L.  
Differential reactivity of 3H-indole styrylcyanines: Intermolecular 4 pi+2 pi cycloaddition vs. proton - shift coupled six - electron electrocyclization  
Tetrahedron, (74): 2999-3006. 2018. 10.1016/j.tet.2018.04.085
- Tidey, J. P.; Zhurov, V. V.; Gianopoulos, C. G.; Hermann, T. S.; Pinkerton, A. A.  
QTAIM Assessment of the Intra- and Intermolecular Bonding in a Bis(nitramido-oxadiazolate) Energetic Ionic Salt at 20 K  
Journal of Physical Chemistry A, (122): 9676-9687. 2018. 10.1021/acs.jpca.8b10065
- Tighadouini, S.; Benabbes, R.; Tillard, M.; Eddike, D.; Haboubi, K.; Karrouchi, K.; Radi, S.  
Synthesis, crystal structure, DFT studies and biological activity of (Z)-3-(3-bromophenyl)-1-(1,5-dimethyl-1H-pyrazol-3-yl)-3-hydroxyprop-2-en -1-one  
Bmc Chemistry, (12) 2018. 10.1186/s13065-018-0492-4
- Tighadouini, S.; Benabbes, R.; Tillard, M.; Eddike, D.; Haboubi, K.; Karrouchi, K.; Radi, S.  
Synthesis, crystal structure, DFT studies and biological activity of (Z)-3-(3-bromophenyl)-1-(1,5-dimethyl-1H-pyrazol-3-yl)-3-hydroxyprop-2-e n-1-one  
Chemistry Central Journal, (12) 2018. 10.1186/s13065-018-0492-4
- Tikhonov, D. S.; Sharapa, D. I.; Otlyotov, A. A.; Solyankin, P. M.; Rykov, A. N.; Shkurinov, A. P.; Grikina, O. E.; Khaikin, L. S.  
Nitroxoline Molecule: Planar or Not? A Story of Battle between pi-pi Conjugation and Interatomic Repulsion  
Journal of Physical Chemistry A, (122): 1691-1701. 2018. 10.1021/actipca.7b11364
- Timofeeva, D. S.; Mayer, R. J.; Mayer, P.; Ofial, A. R.; Mayr, H.  
Which Factors Control the Nucleophilic Reactivities of Enamines?  
Chemistry-a European Journal, (24): 5901-5910. 2018. 10.1002/chem.201705962

- Tokatli, A.; Ucun, F.; Sutcu, K.; Osmanoglu, Y. E.; Osmanoglu, S.  
Spectral analysis and quantum chemical studies of chair and twist-boat conformers of cycloheximide in gas and solution phases  
*Journal of Molecular Structure*, (1154): 428-436. 2018. 10.1016/j.molstruc.2017.10.037
- Tomsu, G.; Mastalir, M.; Pittenauer, E.; Stoger, B.; Allmaier, G.; Kirchner, K.  
Ligand-Enforced Switch of the Coordination Mode in Low-Valent Group 6 Carbonyl Complexes Containing Pyrimidine-Based Bisphosphines  
*Organometallics*, (37): 1919-1926. 2018. 10.1021/acs.organomet.8b00192
- Tondreau, A. M.; Duignan, T. J.; Stein, B. W.; Fleischauer, V. E.; Autschbach, J.; Batista, E. R.; Boncella, J. M.; Ferrier, M. G.; Kozimor, S. A.; Mocko, V.; Neidig, M. L.; Cary, S. K.; Yang, P.  
A Pseudotetrahedral Uranium(V) Complex  
*Inorganic Chemistry*, (57): 8106-8115. 2018. 10.1021/acs.inorgchem.7b03139
- Topfer, K.; Tremblay, J. C.  
First-Principle Investigations of the Interaction between CO and O-2 with Group 11 Atoms on a Defect-Free MgO(001) Surface  
*Journal of Physical Chemistry A*, (122): 2307-2317. 2018. 10.1021/acs.jpca.8b00647
- Torabi, V.; Kargar, H.; Akbari, A.; Behjatmanesh-Ardakani, R.; Rudbari, H. A.; Tahir, M. N.  
Nickel(II) complex with an asymmetric tetradeятate Schiff base ligand: synthesis, characterization, crystal structure, and DFT studies  
*Journal of Coordination Chemistry*, (71): 3748-3762. 2018. 10.1080/00958972.2018.1521967
- Tornheim, A.; Sahore, R.; He, M.; Croy, J. R.; Zhang, Z. C.  
Preformed Anodes for High-Voltage Lithium-Ion Battery Performance: Fluorinated Electrolytes, Crosstalk, and the Origins of Impedance Rise  
*Journal of the Electrochemical Society*, (165): A3360-A3368. 2018. 10.1149/2.0611814jes
- Toupkanloo, H. A.; Rahmani, Z.  
An in-depth study on noncovalent stacking interactions between DNA bases and aromatic drug fragments using DFT method and AIM analysis: conformers, binding energies, and charge transfer  
*Applied Biological Chemistry*, (61): 209-226. 2018. 10.1007/s13765-018-0348-6
- Traesel, H. J.; Olivato, P. R.; Valenca, J.; Rodrigues, D. N. S.; Zukerman-Schpector, J.; Dal Colle, M.  
Conformational analysis of some 4'-substituted 2-(phenylselanyl)-2-(methoxy)- acetophenones  
*Journal of Molecular Structure*, (1157): 29-39. 2018. 10.1016/j.molstruc.2017.12.040
- Tran, V.; Allen, K. E.; Chavez, M. G.; Aaron, C.; Dumais, J. J.; York, J. T.; Brown, E. C.  
Solution and solid-state characterization of Zn(II) complexes containing a new tridentate N<sub>2</sub>S ligand  
*Polyhedron*, (147): 131-141. 2018. 10.1016/j.poly.2018.03.008

Transue, W. J.; Yang, J. Y.; Nava, M.; Sergeyev, I. V.; Barnum, T. J.; McCarthy, M. C.; Cummins, C. C.

Synthetic and Spectroscopic Investigations Enabled by Modular Synthesis of Molecular Phosphaalkyne Precursors

Journal of the American Chemical Society, (140): 17985-17991. 2018. 10.1021/jacs.8b09845

Trevino, M. A.; Pantoja-Uceda, D.; Menendez, M.; Gomez, M. V.; Mompean, M.; Laurents, D. V.

The Singular NMR Fingerprint of a Polyproline II Helical Bundle

Journal of the American Chemical Society, (140): 16988-17000. 2018. 10.1021/jacs.8b05261

Tri, N. N.; Carvalho, J. P.; Dordio, A. V.; Nguyen, M. T.; Trung, N. T.

Insight into the adsorption of chloramphenicol on a vermiculite surface

Chemical Physics Letters, (699): 107-114. 2018. 10.1016/j.cplett.2018.03.040

Triewel, R. C.; Scheiner, S.

Crystallographic and Computational Characterization of Methyl Tetrel Bonding in S-Adenosylmethionine-Dependent Methyltransferases

Molecules, (23) 2018. 10.3390/molecules23112965

Tsipis, A. C.

Interaction of Elemental Mercury with a Diverse Series of pi-Organic Substrates Probed by Computational Methods: Is Mercury Fixation Possible?

ACS Earth and Space Chemistry, (2): 451-+. 2018. 10.1021/acsearthspacechem.7b00122

Tsubomoto, Y.; Hayashi, S.; Nakanishi, W.; Mapp, L. K.; Coles, S. J.

High-resolution X-ray diffraction determination of the electron density of 1-(8-PhSC<sub>10</sub>H<sub>6</sub>SPh-8')-1' with the QTAIM approach: evidence for S-4 sigma(4c-6e) at the naphthalene peri-positions

RSC Advances, (8): 9651-9660. 2018. 10.1039/c7ra13636f

Tsukasaki, H.; Fukuda, W.; Morimoto, H.; Arai, T.; Mori, S.; Hayashi, A.; Tatsumisago, M.

Thermal behavior and microstructures of cathodes for liquid electrolyte-based lithium batteries

Scientific Reports, (8) 2018. 10.1038/s41598-018-34017-2

Tsuruoka, K.; Koyasu, K.; Hirabayashi, S.; Ichihashi, M.; Tsukuda, T.

Size-Dependent Polymorphism in Aluminum Carbide Cluster Anions AlnC<sub>2</sub>-: Formation of Acetylide-Containing Structures

Journal of Physical Chemistry C, (122): 8341-8347. 2018. 10.1021/acs.jpcc.7b12767

Tulyabaev, A. R.; Bikmukhametov, K. S.; Mescheryakova, E. S.; Makhmudiyarova, N. N.; Rakhimov, R. S.; Khalilov, L. M.

What is responsible for conformational diversity in single-crystal tetraoxazaspiroalkanes? X-Ray, DFT, and AIM approaches

Crystengcomm, (20): 3207-3217. 2018. 10.1039/c8ce00481a

Turnbull, D.; Kostiuk, N.; Wetmore, S. D.; Gerken, M.

Syntheses, characterisation, and computational studies of tungsten hexafluoride adducts with pyridine and its derivatives

Journal of Fluorine Chemistry, (215): 1-9. 2018. 10.1016/j.jfluchem.2018.08.007

Tuscher, L.; Helling, C.; Wolpe, C.; Frank, W.; Nizovtsev, A. S.; Schulz, S.

A General Route to Metal-Substituted Dipnictenes of the Type L(X)M (2)E-2

Chemistry-a European Journal, (24): 3241-3250. 2018. 10.1002/chem.201705233

Tuttle, W. D.; Harris, J. P.; Zheng, Y.; Breckenridge, W. H.; Wright, T. G.

Hybridization and Covalency in the Group 2 and Group 12 Metal Cation/Rare Gas Complexes

Journal of Physical Chemistry A, (122): 7679-7703. 2018. 10.1021/acs.jpca.8b07139

Uhl, W.; Honacker, C.; Lawrence, N.; Hepp, A.; Schurmann, L.; Layh, M.

Hydroalumination of Oligoalkynylgermanes and -digermanes - Reactions with Heterocumulenes by Al-C or Ge-C Bond Activation and Formation of a Hexazenedialuminum Complex

Zeitschrift fur Anorganische und Allgemeine Chemie, (644): 945-955. 2018.

10.1002/zaac.201800159

Uludag, N.; Serdaroglu, G.

An improved synthesis, spectroscopic (FT-IR, NMR) study and DFT computational analysis (IR, NMR, UV-Vis, MEP diagrams, NBO, NLO, FMO) of the 1,5-methanoazocino 4,3-b indole core structure

Journal of Molecular Structure, (1155): 548-560. 2018. 10.1016/j.molstruc.2017.11.032

Uludag, N.; Serdaroglu, G.; Yinanc, A.

A novel synthesis of octahydropyrido 3,2-c carbazole framework of aspidospermidine alkaloids and a combined computational, FT-IR, NMR, NBO, NLO, FMO, MEP study of the cis-4a-Ethyl-1(2hydroxyethyl)-2,3,4,4a,5,6,7,11c-octahydro-1H-pyrido 3,2 -c carbazole

Journal of Molecular Structure, (1161): 152-168. 2018. 10.1016/j.molstruc.2018.02.046

Ungati, H.; Govindaraj, V.; Muges, G.

The Remarkable Effect of Halogen Substitution on the Membrane Transport of Fluorescent Molecules in Living Cells

Angewandte Chemie-International Edition, (57): 8989-8993. 2018. 10.1002/anie.201804128

Unsleber, J. P.; Neugebauer, J.; Morris, R. H.

DFT methods applied to answer the question: how accurate is the ligand acidity constant method for estimating the pK(a) of transition metal hydride complexes MHXL4 when X is varied?

Dalton Transactions, (47): 2739-2747. 2018. 10.1039/c7dt03473c

Upadhyaya, P.; Devi, T. G.

Raman bandshape analysis and DFT study of C=O and C-H stretching modes of NN-Dibutyl formamide in DMSO solvent

Vibrational Spectroscopy, (96): 110-117. 2018. 10.1016/j.vibspec.2018.03.006

Usui, K.; Haines, B. E.; Musaev, D. G.; Sarpong, R.

Understanding Regiodivergence in a Pd(II)-Mediated Site-Selective C-H Alkynylation

ACS Catalysis, (8): 4516-4527. 2018. 10.1021/acscatal.8b01116

Uzunova, E. L.

Theoretical study of nitrogen dioxide and nitric oxide co-adsorption and DeNO(x) reaction on Cu-SAPO-34 and Cu-SSZ-13 in presence of Bronsted acid sites

Molecular Catalysis, (447): 47-55. 2018. 10.1016/j.mcat.2018.01.003

Vafazadeh, R.; Namazian, M.; Shahpoori-Arani, B.; Willis, A. C.; Carr, P. D.

Synthesis, X-ray Structural Characterization, and DFT Calculations of Mononuclear Nickel(II) Complexes Containing Diamine and Methacrylate Ligands

Acta Chimica Slovenica, (65): 372-379. 2018. 10.17344/acsi.2017.4096

Valenca, J.; Rodrigues, D. N. S.; Olivato, P. R.; Dal Colle, M.

Spectroscopic and theoretical studies of some 2-(2'-haloacetyl)-5-substituted: 1-Methylpyrrole, furan and thiophene

Journal of Molecular Structure, (1151): 301-314. 2018. 10.1016/j.molstruc.2017.09.055

Vanasundari, K.; Balachandran, V.; Kavimani, M.; Narayana, B.

Molecular docking, vibrational, structural, electronic and optical studies of {4(2,6)dichlorophenyl amino 2-methylidene 4-oxobutanoic acid and 4-(2,5)). dichlorophenyl amino 2-methylidene 4-oxobutanoic acid A comparative study

Journal of Molecular Structure, (1155): 21-38. 2018. 10.1016/j.molstruc.2017.11.002

Vandezande, J. E.; Schaefer, H. F.

CO<sub>2</sub> Reduction Pathways on MnBr(N-C)(CO)(3) Electrocatalysts

Organometallics, (37): 337-342. 2018. 10.1021/acs.organomet.7b00743

Vannay, L.; Meyer, B.; Petraglia, R.; Sforazzini, G.; Ceriotti, M.; Corminboeuf, C.

Analyzing Fluxional Molecules Using DORI

Journal of Chemical Theory and Computation, (14): 2370-2379. 2018. 10.1021/acs.jctc.7b01176

Vasilchenko, D.; Vorobieva, S.; Baidina, I.; Piryazev, D.; Tsipis, A.; Korenev, S.

Structure and properties of a rhodium(III) pentanitrito complex embracing uni- and bidentate nitrito ligands

Polyhedron, (147): 69-74. 2018. 10.1016/j.poly.2018.03.017

Vasilchenko, D. B.; Tkachev, S. V.; Tsipis, A. C.

Aquanitrito Complexes of Palladium, Rhodium, and Platinum: A Comparative N-15 NMR and DFT Study

European Journal of Inorganic Chemistry: 627-639. 2018. 10.1002/ejic.201701140

Vasiliu, M.; Hill, J. G.; Peterson, K. A.; Dixon, D. A.

Structures and Heats of Formation of Simple Alkaline Earth Metal Compounds II: Fluorides, Chlorides, Oxides, and Hydroxides for Ba, Sr, and Ra

Journal of Physical Chemistry A, (122): 316-327. 2018. 10.1021/acs.jpca.7b09056

Vasquez-Espinal, A.; Palacio-Rodriguez, K.; Ravell, E.; Orozco-Ic, M.; Barroso, J.; Pan, S.; Tiznado, W.; Merino, G.

E5M7+ (E=C-Pb, M=Li-Cs): A Source of Viable Star-Shaped Clusters

Chemistry-an Asian Journal, (13): 1751-1755. 2018. 10.1002/asia.201800654

Vekeman, J.; Cuesta, I. G.; Faginas-Lago, N.; Wilson, J.; Sanchez-Marin, J.; de Meras, A. S.

Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks

Physical Chemistry Chemical Physics, (20): 25518-25530. 2018. 10.1039/c8cp03652g

Vektariene, A.

The Bonding Nature of Cyclometalated Ru Complex: How DFT Study Revealing the Dewar-Chatt-Duncanson Model Relates to the Molecular Properties

Chemistryselect, (3): 10750-10761. 2018. 10.1002/slct.201802330

Vektariene, A.

THE TRANSITION METAL TO LIGAND BONDING NATURE: A QUANTUM CHEMICAL STUDY OF pi-ALLYL-RUTHENACYCLE MOLECULE

Lithuanian Journal of Physics, (58): 232-245. 2018.

Venkatesan, V.

Ab Initio Studies on the Interaction Between Copper(I) and 5-Nitrotetrazolate Anion

Defence Science Journal, (68): 12-18. 2018. 10.14429/dsj.68.10409

Venkatesh, G.; Kamal, C.; Vennila, P.; Govindaraju, M.; Mary, Y. S.; Armakovic, S.; Armakovic, S. J.; Kaya, S.; Panicker, C. Y.

Molecular dynamic simulations, ALIE surface, Fukui functions geometrical, molecular docking and vibrational spectra studies of tetra chloro p and m-xylene

Journal of Molecular Structure, (1171): 253-267. 2018. 10.1016/j.molstruc.2018.06.001

Vennila, P.; Govindaraju, M.; Venkatesh, G.; Kamal, C.; Mary, Y. S.; Panicker, C. Y.; Kaya, S.; Armakovic, S.; Armakovic, S. J.

A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene - A frequently used benzene derivative

Journal of Molecular Structure, (1151): 245-255. 2018. 10.1016/j.molstruc.2017.09.049

Verhoeven, D. G. A.; van Wiggen, M. A. C.; Kwakernaak, J.; Lutz, M.; Gebbink, R.; Moret, M. E.

Periodic Trends in the Binding of a Phosphine-Tethered Ketone Ligand to Fe, Co, Ni, and Cu

Chemistry-a European Journal, (24): 5163-5172. 2018. 10.1002/chem.201703254

Verma, K.; Viswanathan, K. S.

"A Tale of Two Structures": The Stacks and Ts of Borazine and Benzene Hetero and Homo Dimers

Chemistryselect, (3): 864-873. 2018. 10.1002/slct.201703005

Verma, P. L.; Gejji, S. P.

Electronic structure, spectral characteristics and physicochemical properties of linear, branched and cyclic alkyl group substituted 1-alkyl-3-butylimidazolium cation based ionic liquids

Journal of Molecular Liquids, (251): 394-406. 2018. 10.1016/j.molliq.2017.12.040

Verma, P. L.; Gejji, S. P.

Modeling protic dicationic ionic liquids based on quaternary ammonium, imidazolium or pyrrolidinium cations and bis(trifluoromethanesulfonyl)imide anion: Structure and spectral characteristics

Journal of Molecular Graphics & Modelling, (85): 304-315. 2018. 10.1016/j.jmgm.2018.09.010

Verma, P. L.; Gejji, S. P.

Unveiling Noncovalent Interactions in Imidazolium, Pyrrolidinium, or Quaternary Ammonium Cation and Acetate Anion Based Protic Ionic Liquids: Structure and Spectral Characteristics

Journal of Physical Chemistry A, (122): 6225-6235. 2018. 10.1021/acs.jpca.8b04303

Vibhute, A. M.; Priyakumar, U. D.; Ravi, A.; Sureshan, K. M.

Model molecules to classify CH center dot center dot center dot O hydrogen-bonds

Chemical Communications, (54): 4629-4632. 2018. 10.1039/c8cc01653d

Vicha, J.; Komorovsky, S.; Repisky, M.; Marek, R.; Straka, M.

Relativistic Spin-Orbit Heavy Atom on the Light Atom NMR Chemical Shifts: General Trends Across the Periodic Table Explained

Journal of Chemical Theory and Computation, (14): 3025-3039. 2018. 10.1021/acs.jctc.8b00144

Viesser, R. V.; Ducati, L. C.; Tormena, C. F.; Autschbach, J.

The halogen effect on the C-13 NMR chemical shift in substituted benzenes

Physical Chemistry Chemical Physics, (20): 11247-11259. 2018. 10.1039/c8cp01249k

Villalba, C. M. A.; Rozada, T. D.; dos Santos, F. S.; Scorsin, L.; Garcia, J. R.; Fiorin, B. C.

Experimental and Theoretical Study of the Reaction Kinetics of 2,5-Dimethylterephthalonitrile Bromination Compared to 1,4-Dimethylbenzene Bromination

Synthesis-Stuttgart, (50): 1259-1263. 2018. 10.1055/s-0036-1591750

Villani, G.

Quantum Mechanical Investigation of the G-Quadruplex Systems of Human Telomere

ACS Omega, (3): 9934-9944. 2018. 10.1021/acsomega.8b01678

- Villaverde, J. J.; Sandin-Espana, P.; Alonso-Prados, J. L.; Lamsabhi, A.; Alcami, M.  
Computational Study of the Structure and Degradation Products of Alloxydim Herbicide  
Journal of Physical Chemistry A, (122): 3909-3918. 2018. 10.1021/acs.jpca.8b00865
- Viola, E.; Donzello, M. P.; Ercolani, C.; Rizzoli, C.; Lever, A. B. P.  
Synthesis and structure of rare zwitterionic complexes involving the presence of N(py)MCl<sub>3</sub>-moieties (M = Pt(II), Pd(II))  
Inorganica Chimica Acta, (480): 101-107. 2018. 10.1016/j.ica.2018.04.031
- Vogt, N.; Marochkin, II; Rykov, A. N.  
Experiment and theory at the convergence limit: accurate equilibrium structure of picolinic acid by gas-phase electron diffraction and coupled-cluster computations  
Physical Chemistry Chemical Physics, (20): 9787-9795. 2018. 10.1039/c8cp00310f
- Voityuk, A. A.; Stasyuk, A. J.; Vyboishchikov, S. F.  
A simple model for calculating atomic charges in molecules  
Physical Chemistry Chemical Physics, (20): 23328-23337. 2018. 10.1039/c8cp03764g
- Vokacova, Z. S.; Turel, I.; Burda, J. V.  
Exploration of selected electronic characteristics of half-sandwich organoruthenium(II) beta-diketonate complexes  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3598-7
- von Szentpaly, L.  
Eliminating Symmetry Problems in Electronegativity Equalization and Correcting Self-Interaction Errors in Conceptual DFT  
Journal of Computational Chemistry, (39): 1949-1969. 2018. 10.1002/jcc.25356
- Vu, K. B.; Vu, V. V.; Thu, H. P. T.; Giang, H. N.; Tam, N. M.; Ngo, S. T.  
Conjugated polymers: A systematic investigation of their electronic and geometric properties using density functional theory and semi-empirical methods  
Synthetic Metals, (246): 128-136. 2018. 10.1016/j.synthmet.2018.10.007
- Wagner, J. P.; McDonald, D. C.; Duncan, M. A.  
An Argon-Oxygen Covalent Bond in the ArOH<sup>+</sup> Molecular Ion  
Angewandte Chemie-International Edition, (57): 5081-5085. 2018. 10.1002/anie.201802093
- Wahab, F. F. A.; Shamsuddin, M.; Bulat, K. H. K.; Ismail, N.  
Structural, density functional computational studies and antibacterial screening on N,N'-bis-(4-hydroxy-alpha-methylsalicylidene)ethylenediamine nickel (II) complex  
Polyhedron, (156): 165-173. 2018. 10.1016/j.poly.2018.09.016
- Wang, B.; Wang, X. L.; Li, X. C.; Guo, Z. J.; Zhou, X.; Wu, Y. Q.

The effects of amino substituents on the enhanced ammonia sensing performance of  $\text{PcCo}/\text{rGO}$  hybrids

RSC Advances, (8): 41280-41287. 2018. 10.1039/c8ra07509c

Wang, C.; Jiang, Y. Y.

Theoretical study on abnormal trans-effect of chloride, bromide and iodide ligands in iridium complexes

Computational and Theoretical Chemistry, (1138): 1-6. 2018. 10.1016/j.comptc.2018.05.015

Wang, C.; Xiang, L.; Yang, Y.; Fang, J.; Maron, L.; Leng, X. B.; Chen, Y. F.

Dianionic Carbon-Bridged Scandium-Copper/Silver Heterobimetallic Complexes: Synthesis, Bonding, and Reactivity

Chemistry-a European Journal, (24): 5637-5643. 2018. 10.1002/chem.201706147

Wang, C. H.; Duster, A. W.; Aydintug, B. O.; Zarecki, M. G.; Lin, H.

Chloride Ion Transport by the E-coli CLC Cl-/H<sup>+</sup> Antiporter: A Combined Quantum-Mechanical and Molecular-Mechanical Study

Frontiers in Chemistry, (6) 2018. 10.3389/fchem.2018.00062

Wang, C. W.; Fu, Y. Z.; Zhang, L. N.; Danovich, D.; Shaik, S.; Mo, Y. R.

Hydrogen- and Halogen-Bonds between Ions of like Charges: Are They Anti-Electrostatic in Nature?

Journal of Computational Chemistry, (39): 481-487. 2018. 10.1002/jcc.25068

Wang, G. C.; Freeman, L. A.; Dickie, D. A.; Mokrai, R.; Benko, Z.; Gilliard, R. J.

Highly Reactive Cyclic(alkyl)(amino) Carbene- and N-Heterocyclic Carbene-Bismuth(III) Complexes: Synthesis, Structure, and Computations

Inorganic Chemistry, (57): 11687-11695. 2018. 10.1021/acs.inorgchem.8b01813

Wang, H.; Liu, J.; Wang, W. Z.

Intermolecular and very strong intramolecular C-Se center dot center dot center dot O/N chalcogen bonds in nitrophenyl selenocyanate crystals

Physical Chemistry Chemical Physics, (20): 5227-5234. 2018. 10.1039/c7cp08215k

Wang, H. B.; Liu, Q.; Liu, D. J.; Su, R. Z.; Liu, J. L.; Li, Y. Z.

Computational Prediction of Electronic and Photovoltaic Properties of Anthracene-Based Organic Dyes for Dye-Sensitized Solar Cells

International Journal of Photoenergy, 2018. 10.1155/2018/4764830

Wang, H. L.; Deng, Y. Q.; Zhou, R. J.

Aromatic sulfur compounds oxidation with H<sub>2</sub>O<sub>2</sub> over fully coordinated and defect sites in Ti-beta zeolites: evaluation by density functional theory

Theoretical Chemistry Accounts, (137) 2018. 10.1007/s00214-018-2241-0

Wang, H. L.; Dong, M. M.; Liu, C. B.; Zhang, D. J.

Theoretical insight into the zinc(II)-catalyzed synthesis of 2-indolyltetrahydroquinolines from N-propargylanilines and indoles: cross-dehydrogenative coupling with temporally separated catalytic activity

Catalysis Science & Technology, (8): 1997-2007. 2018. 10.1039/c8cy00181b

Wang, H. L.; Liu, C. B.; Zhang, D. J.

Mechanistic study on the Rh(III)-catalyzed synthesis of indolines via selective O-atom transfer of arylnitrones: Origins of the regioselectivity and the improved yield with pivalic acid additive

Journal of Organometallic Chemistry, (854): 15-26. 2018. 10.1016/j.jorgchem.2017.11.001

Wang, J. J.; Sun, Z.; Meng, L. P.; Zeng, Y. L.

ClEe as the halogen bond acceptor: studies on strong halogen bonds

Structural Chemistry, (29): 503-511. 2018. 10.1007/s11224-017-1047-3

Wang, J. Q.; Du, N.; Chen, H. S.

Structure and stability of Al<sub>n</sub>Mg<sub>m</sub> (n=4-8, m=1-3) clusters: Genetic algorithm and density functional theory approach

Computational and Theoretical Chemistry, (1128): 15-23. 2018. 10.1016/j.comptc.2018.02.006

Wang, L.; Fujii, M.; Yamaji, M.; Okamoto, H.

Fluorescence behaviour of 2-, 3-and 4-amino-1,8-naphthalimides: effects of the substitution positions of the amino functionality on the photophysical properties

Photochemical & Photobiological Sciences, (17): 1319-1328. 2018. 10.1039/c8pp00302e

Wang, Q.; Huang, F.; Jiang, L. H.; Zhang, C. X.; Sun, C. Z.; Liu, J. B.; Chen, D. Z.

Comprehensive Mechanistic Insight into Cooperative Lewis Acid/Cp\*Co-III-Catalyzed C-H/N-H Activation for the Synthesis of Isoquinolin-3-ones

Inorganic Chemistry, (57): 2804-2814. 2018. 10.1021/acs.inorgchem.7b03216

Wang, W. H.; Feng, W. L.; Wang, W. L.; Li, P.

Theoretical Insights into the Electron Capture Behavior of H<sub>2</sub>SO<sub>4</sub> center dot center dot center dot N<sub>2</sub>O Complex: A DFT and Molecular Dynamics Study

Molecules, (23) 2018. 10.3390/molecules23092349

Wang, X. J.; Zhang, G. Z.; Yang, L.; Sharman, E.; Jiang, J.

Material descriptors for photocatalyst/catalyst design

Wiley Interdisciplinary Reviews-Computational Molecular Science, (8) 2018. 10.1002/wcms.1369

Wang, Y.

Maximum bonding fragment orbitals for deciphering complex chemical interactions

Physical Chemistry Chemical Physics, (20): 13792-13809. 2018. 10.1039/c8cp01808a

Wang, Y.; Wei, D. H.; Zhang, W. J.

Recent Advances on Computational Investigations of N-Heterocyclic Carbene Catalyzed Cycloaddition/Annulation Reactions: Mechanism and Origin of Selectivities  
Chemcatchem, (10): 338-360. 2018. 10.1002/cctc.201701119

Wang, Y.; Zeng, X. L.

Addition Reactions of H<sub>2</sub>O to Germastannenes: A Computational Study  
Russian Journal of Physical Chemistry A, (92): 1699-1705. 2018. 10.1134/s0036024418090352

Wang, Y. Y.; Ling, B. P.; Liu, P.; Bi, S. W.

A Reaction Mechanism for Gold-Catalyzed Hydroamination/Cyclization of o-Phenylenediamine and Propargylic Alcohols. A DFT Study  
Organometallics, (37): 3035-3044. 2018. 10.1021/acs.organomet.8b00406

Wang, Z. H.; Wu, Y. J.; Xue, H. H.; Zhou, L. N.; Geng, W. C.; Yi, H. B.; Li, Y. J.

What dictates which ion, I<sup>-</sup> or Br<sup>-</sup>, mediates the growth of cubic Pd nanocrystals?  
Physical Chemistry Chemical Physics, (20): 10997-11002. 2018. 10.1039/c8cp00861b

Wang, Z. T.; Valtchev, V.; Fang, Q. R.; Li, X. M.; Pan, Y. R.

Syntheses, Crystal Structures and Theoretical Calculation of Three-Dimensional Supramolecular Zinc/Manganese Complex  
Chinese Journal of Inorganic Chemistry, (34): 515-524. 2018. 10.11862/cjic.2018.038

Wang, Z. T.; Wang, S. J.; Li, X. M.; Pan, Y. R.

Synthesis, Crystal Structure and Theoretical Calculations of a Cadmium Complex Containing 3-Hydroxybenzoic Acid and 1,4-Bis(imidazol-1-yl)-butane((1))  
Chinese Journal of Structural Chemistry, (37): 467-474. 2018. 10.14102/j.cnki.0254-5861.2011-1786

Wang, Z. X.; Liu, Y.; Zheng, B. S.; Zhou, F. X.; Jiao, Y. C.; Liu, Y.; Ding, X. L.; Lu, T.

A theoretical investigation on Cu/Ag/Au bonding in XH<sub>2</sub>P center dot center dot center dot MY(X = H, CH<sub>3</sub>, F, CN, NO<sub>2</sub>; M = Cu, Ag, Au; Y = F, Cl, Br, I) complexes  
Journal of Chemical Physics, (148) 2018. 10.1063/1.5027605

Wategaonkar, S.; Bhattacherjee, A.

N-H center dot center dot S Interaction Continues To Be an Enigma: Experimental and Computational Investigations of Hydrogen-Bonded Complexes of Benzimidazole with Thioethers  
Journal of Physical Chemistry A, (122): 4313-4321. 2018. 10.1021/acs.jpca.8b01943

Wei, Y. X.; Cheng, J. B.; Yang, S. B.; Xiao, B.; Li, Q. Z.

Influence of substituents and cooperativity in doubly hydrogen-bonded complexes of 2-pyridone and oxalic acid  
Molecular Physics, (116): 1862-1870. 2018. 10.1080/00268976.2018.1459918

Wei, Y. X.; Li, Q. Z.

Comparison for sigma-hole and pi-hole tetrel-bonded complexes involving cyanoacetaldehyde  
Molecular Physics, (116): 222-230. 2018. 10.1080/00268976.2017.1377851

Wei, Y. X.; Li, Q. Z.; Scheiner, S.

The pi-Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer  
Chemphyschem, (19): 736-743. 2018. 10.1002/cphc.201701136

Wei, Z. H.; de Aguirre, A.; Junge, K.; Beller, M.; Jiao, H. J.

Exploring the mechanisms of aqueous methanol dehydrogenation catalyzed by defined PNP Mn and Re pincer complexes under base-free as well as strong base conditions

Catalysis Science & Technology, (8): 3649-3665. 2018. 10.1039/c8cy00746b

Wei, Z. H.; Junge, K.; Beller, M.; Jiao, H. J.

Exploring the activities of vanadium, niobium, and tantalum PNP pincer complexes in the hydrogenation of phenyl-substituted C equivalent to N, C=N, C equivalent to C, C=C, and C=O functional groups

Comptes Rendus Chimie, (21): 303-309. 2018. 10.1016/j.crci.2017.09.001

Weinberger, C.; Hines, R.; Zeller, M.; Rosokha, S. V.

Continuum of covalent to intermolecular bonding in the halogen-bonded complexes of 1,4-diazabicyclo 2.2.2 octane with bromine-containing electrophiles

Chemical Communications, (54): 8060-8063. 2018. 10.1039/c8cc04629h

Weinhold, F.; Glendening, E. D.

Comment on "Natural Bond Orbitals and the Nature of the Hydrogen Bond"

Journal of Physical Chemistry A, (122): 724-732. 2018. 10.1021/acs.jpca.7b08165

Weinhold, F.

Theoretical Prediction of Robust Second-Row Oxyanion Clusters in the Metastable Domain of Antielectrostatic Hydrogen Bonding

Inorganic Chemistry, (57): 2035-2044. 2018. 10.1021/acs.inorgchem.7b02943

Weis, P.; Kratzert, D.; Krossing, I.

Silver Coordination Chemistry of the Weakly Basic Cage As<sub>4</sub>S<sub>4</sub>

European Journal of Inorganic Chemistry: 3203-3212. 2018. 10.1002/ejic.201800430

Welz, E.; Bohnke, J.; Dewhurst, R. D.; Braunschweig, H.; Engels, B.

Unravelling the Dramatic Electrostructural Differences Between N-Heterocyclic Carbene- and Cyclic (Alkyl)(amino)carbene-Stabilized Low-Valent Main Group Species

Journal of the American Chemical Society, (140): 12580-12591. 2018. 10.1021/jacs.8b07644

Wen, M.; Li, Z. Z.; Li, A. Y.

Noble gas inserted compounds of borazine and its derivative B<sub>3</sub>N<sub>3</sub>R<sub>6</sub>: structures and bonding

Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3860-z

Weske, S.; Hardin, R. A.; Auth, T.; O'Hair, R. A. J.; Koszinowski, K.; Ogle, C. A.  
Argentate(I) and (III) complexes as intermediates in silver-mediated cross-coupling reactions  
Chemical Communications, (54): 5086-5089. 2018. 10.1039/c8cc01707g

Wiberg, K. B.; Rablen, P. R.  
Atomic Charges  
Journal of Organic Chemistry, (83): 15463-15469. 2018. 10.1021/acs.joc.8b02740

Wiberg, K. B.; Rablen, P. R.  
Methoxymethane C-O Bond Strengths: Do Their Changes Result from Hyperconjugation or Polar Effects?  
Journal of Physical Chemistry A, (122): 6021-6025. 2018. 10.1021/acs.jpca.8b03923

Wiesemann, M.; Hoge, B.  
Pentafluoroethylated Compounds of Silicon, Germanium and Tin  
Chemistry-a European Journal, (24): 16457-16471. 2018. 10.1002/chem.201801292

Wilson, H. H.; Koellner, C. A.; Hannan, Z. M.; Endy, C. B.; Bezpalko, M. W.; Piro, N. A.; Kassel, W. S.; Sonntag, M. D.; Graves, C. R.  
Synthesis and Characterization of Neutral Ligand alpha-Diirnine Complexes of Aluminum with Tunable Redox Energetics  
Inorganic Chemistry, (57): 9622-9633. 2018. 10.1021/acs.inorgchem.8b00045

Wilson, R. E.; De Sio, S.; Vallet, V.  
Protactinium and the intersection of actinide and transition metal chemistry  
Nature Communications, (9) 2018. 10.1038/s41467-018-02972-z

Wilson, R. J.; Hastreiter, F.; Reiter, K.; Buschelberger, P.; Wolf, R.; Gschwind, R. M.; Weigend, F.; Dehnen, S.  
Co@Sn<sub>6</sub>Sb<sub>6</sub> (3-) : An Off-Center Endohedral 12-Vertex Cluster  
Angewandte Chemie-International Edition, (57): 15359-15363. 2018. 10.1002/anie.201807180

Windsor, I. W.; Palte, M. J.; Lukesh, J. C.; Gold, B.; Forest, K. T.; Raines, R. T.  
Sub-picomolar Inhibition of HIV-1 Protease with a Boronic Acid  
Journal of the American Chemical Society, (140): 14015-14018. 2018. 10.1021/jacs.8b07366

Witteman, L.; Evers, T.; Lutz, M.; Moret, M. E.  
A Free Silanide from Nucleophilic Substitution at Silicon(II)  
Chemistry-a European Journal, (24): 12236-12240. 2018. 10.1002/chem.201801435

Wozniak, D. I.; Sabbers, W. A.; Weerasiri, K. C.; Dinh, L. V.; Quenzer, J. L.; Hicks, A. J.; Dobereiner, G. E.  
Comparing Interactions of a Three-Coordinate Pd Cation with Common Weakly Coordinating Anions

Organometallics, (37): 2376-2385. 2018. 10.1021/acs.organomet.8b00356

Wu, C. H.; Zhang, Y.; van Rickley, K.; Wu, J. I.

Aromaticity gain increases the inherent association strengths of multipoint hydrogen-bonded arrays

Chemical Communications, (54): 3512-3515. 2018. 10.1039/c8cc00422f

Wu, H. M.; Luo, Z. X.

Chlorine-passivated superatom Al-37 clusters for nonlinear optics

Science China-Chemistry, (61): 1619-1623. 2018. 10.1007/s11426-018-9316-4

Wu, H. M.; Yuan, C. Q.; Zeng, C. H.; Luo, Z. X.

Quantum Tunneling Tautomer of N,N-Dimethyl-p-toluidine Dehydrogenates Identified by Deep-UV Laser Ionization Mass Spectroscopy

ACS Omega, (3): 10743-10747. 2018. 10.1021/acsomega.8b01840

Wu, H. M.; Yuan, C. Q.; Zhang, H. Y.; Yang, G. H.; Cui, C. N.; Yang, M. Z.; Bian, W. S.; Fu, H. B.; Luo, Z. X.; Yao, J. N.

Ultrafast Deep-Ultraviolet Laser Ionization Mass Spectrometry Applicable To Identify Phenylenediamine Isomers

Analytical Chemistry, (90): 10635-10640. 2018. 10.1021/acs.analchem.8b03167

Wu, J. J.; Liu, X.; Hao, Y. L.; Chen, H. J.; Su, P. F.; Wu, W.; Zhu, J.

sigma-Aromaticity in a Fully Unsaturated Ring

Chemistry-an Asian Journal, (13): 3691-3696. 2018. 10.1002/asia.201801279

Wu, Q. Y.; Cheng, Z. P.; Lan, J. H.; Wang, C. Z.; Chai, Z. F.; Gibson, J. K.; Shi, W. Q.

Insight into the nature of M-C bonding in the lanthanide/actinide-biscarbene complexes: a theoretical perspective

Dalton Transactions, (47): 12718-12725. 2018. 10.1039/c8dt02702a

Wu, Q. Y.; Su, H.; Wang, H. Y.; Wang, H.

Ab initio calculations, structure, NBO and NCI analyses of X-H . . . pi interactions

Chemical Physics Letters, (693): 202-209. 2018. 10.1016/j.cplett.2018.01.015

Wu, X.; Zhao, L. L.; Jiang, D. D.; Fernandez, I.; Berger, R.; Zhou, M. F.; Frenking, G.

Barium as Honorary Transition Metal in Action: Experimental and Theoretical Study of Ba(CO)(+) and Ba(CO)(-)

Angewandte Chemie-International Edition, (57): 3974-3980. 2018. 10.1002/anie.201713002

Wu, Z.; Feng, R. J.; Xu, J.; Lu, Y.; Lu, B.; Yang, T.; Frenking, G.; Trabelsi, T.; Francisco, J. S.; Zeng, X. Q.

Photoinduced Sulfur-Nitrogen Bond Rotation and Thermal Nitrogen Inversion in Heterocumulene OSNSO

Journal of the American Chemical Society, (140): 1231-1234. 2018. 10.1021/jacs.7b12622

Xi, H. W.; Goh, H. W.; Xu, J. Z.; Lee, P. P. F.; Lim, K. H.

Theoretical design and exploration of novel high energy density materials based on silicon  
Journal of Energetic Materials, (36): 291-301. 2018. 10.1080/07370652.2017.1399943

Xia, J. J.; Asiri, A. M.; Alamry, K. A.; Wu, P.; Huang, Z. H.

Pyrolysis of (thio)carbonates via computation analysis

Journal of Theoretical & Computational Chemistry, (17) 2018. 10.1142/s0219633618500414

Xia, L.; Wang, W. Z.; Liu, S.; Jia, X. G.; Zhang, Y. H.; Li, L. L.; Wu, Y.; Su, B. Y.; Geng, S. B.; Fan, W.

New Coordination Complexes Based on the 2,6-bis 1-(Phenylimino)ethyl Pyridine Ligand:  
Effective Catalysts for the Synthesis of Propylene Carbonates from Carbon Dioxide and Epoxides  
Molecules, (23) 2018. 10.3390/molecules23092304

Xiang, G. L.; Tang, Y.; Liu, Z. G.; Zhu, W.; Liu, H. T.; Wang, J.; Zhong, G. M.; Li, J.; Wang, X.

Probing Ligand-Induced Cooperative Orbital Redistribution That Dominates Nanoscale Molecule-Surface Interactions with One-Unit-Thin TiO<sub>2</sub> Nanosheets  
Nano Letters, (18): 7809-7815. 2018. 10.1021/acs.nanolett.8b03572

Xiang, Y.; Camarada, M. B.; Wen, Y. P.; Wu, H.; Chen, J. Y.; Li, M. F.; Liao, X. N.

Simple voltammetric analyses of ochratoxin A in food samples using highly-stable and anti-fouling black phosphorene nanosensor  
Electrochimica Acta, (282): 490-498. 2018. 10.1016/j.electacta.2018.06.055

Xie, H. J.; Zhang, Y. T.; Xiang, C. Y.; Li, Y.; Fan, T.; Lei, Q. F.; Fang, W. J.

Non-innocent PNN ligand is important for CO oxidation by N<sub>2</sub>O catalyzed by a (PNN)Ru-H pincer complex: insights from DFT calculations

Dalton Transactions, (47): 15324-15330. 2018. 10.1039/c8dt03304h

Xie, L. L.; Liu, L. F.; Wang, W. M.; Ma, Z.; Xu, L. Q.; Zhao, X.; Wang, H. F.

The Structures, Spectroscopic Properties, and Photodynamic Reactions of Three RuCl(QN)NO (-) Complexes (HQN=8-Hydroxyquinoline and Its Derivatives) as Potential NO-Donating Drugs  
Bioinorganic Chemistry and Applications, 2018. 10.1155/2018/7029376

Xie, Q.; Sun, T. T.; Zhu, J.

Probing the Strongest Aromatic Cyclopentadiene Ring by Hyperconjugation  
Organometallics, (37): 3219-3224. 2018. 10.1021/acs.organomet.8b00571

Xie, X. H.; Feng, X. H.; Zhao, X. W.

The effects of electronic structures of four benzodithiophene-based copolymers on their photovoltaic performances

Computational and Theoretical Chemistry, (1145): 28-36. 2018. 10.1016/j.comptc.2018.10.005

Xie, X. H.; Zhao, X. W.; Li, M.

Theoretical Study on the Photoelectric Properties of a Class of Copolymers Based on Benzodithiophene for Solar Cells

International Journal of Polymer Science, 2018. 10.1155/2018/3270313

Xing, M. M.; Guo, L.; Hao, Z. J.

Theoretical study of the single noble metal stabilized on metal oxide clusters catalyze the water-gas shift reaction

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25767

Xing, Y. Y.; Liu, J. B.; Sun, C. Z.; Huang, F.; Chen, D. Z.

Mechanistic Exploration of Cp<sup>\*</sup>Co-III/Rh-III-Catalyzed Carboamination/Olefination of N-Phenoxyacetamides with Alkenes

Inorganic Chemistry, (57): 10726-10735. 2018. 10.1021/acs.inorgchem.8b01352

Xing, Y. Y.; Liu, J. B.; Sun, C. Z.; Huang, F.; Chen, D. Z.

Mechanistic Exploration of the Competition Relationship between a Ketone and C=C, C=N, or C=S Bond in the Rh(III)-Catalyzed Carbocyclization Reactions

Journal of Organic Chemistry, (83): 4545-4553. 2018. 10.1021/acs.joc.8b00292

Xiong, R.; Die, D.; Xu, Y. G.; Zheng, B. X.; Fu, Y. C.

Probing the structural, electronic and magnetic properties of AgnSc (n=1-16) clusters

Physical Chemistry Chemical Physics, (20): 15824-15834. 2018. 10.1039/c8cp02605j

Xu, B.; Li, L.; Shi, P. P.; Yu, W. J.; Zhao, J.; Wang, X. F.; Andrews, L.

Matrix-Infrared Spectra and Structures of HM-SiH<sub>3</sub> (M = Ge, Sn, Pb, Sb, Bi, Te Atoms)

Journal of Physical Chemistry A, (122): 81-88. 2018. 10.1021/acs.jpca.7b09635

Xu, B.; Li, L.; Yu, W. J.; Huang, T. F.; Wang, X. F.

Matrix Infrared Spectra and Theoretical Calculations of Fluoroboryl Complexes F<sub>2</sub>B-MF (M = C, Si, Ge, Sn and Pb)

Journal of Physical Chemistry A, (122): 7301-7311. 2018. 10.1021/acs.jpca.8b04437

Xu, H.; Zhu, Y. Y.; Guo, P.; Liu, C. M.; Shan, J. K.; Tang, M. S.

Mechanisms of phosphine-catalyzed 4+3 annulation of allenotes with C, N-cyclic azomethine imines: A DFT investigation

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25626

Xu, H.; Zhu, Z. H.; Guo, Y. E.; Liu, C. M.; Zhang, W. J.; Zhu, Y. Y.; Wang, Y. L.; Tang, M. S.

A DFT study on N-heterocyclic carbene catalyzed 4+2 annulation reaction with in situ generated heterocyclic ortho-quinodimethane: Mechanism, origin of enantioselectivity and role of catalyst

Tetrahedron, (74): 1009-1015. 2018. 10.1016/j.tet.2018.01.030

Xu, H. L.; Cheng, J. B.; Li, H. B.; Yang, X.; Li, Q. Z.

Tetrel bonds between PhSiF<sub>3</sub>/PhTH<sub>3</sub> (T = Si, Ge, Sn) and H(3)ZO (Z = N, P, As): A pentacoordinate silicon (IV) complex

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25660

Xu, H. L.; Li, Q. Z.; Scheiner, S.

Effect of Magnesium Bond on the Competition Between Hydrogen and Halogen Bonds and the Induction of Proton and Halogen Transfer

Chemphyschem, (19): 1456-1464. 2018. 10.1002/cphc.201800102

Xu, J.; Perraud, V.; Finlayson-Pitts, B. J.; Gerber, R. B.

Uptake of water by an acid-base nanoparticle: theoretical and experimental studies of the methanesulfonic acid-methylamine system

Physical Chemistry Chemical Physics, (20): 22249-22259. 2018. 10.1039/c8cp03634a

Xu, J.; Wu, Z.; Wan, H. B.; Deng, G. H.; Lu, B.; Eckhardt, A. K.; Schreiner, P. R.; Trabelsi, T.; Francisco, J. S.; Zeng, X. Q.

Phenylsulfinyl Radical: Gas -Phase Generation, Photoisomerization, and Oxidation

Journal of the American Chemical Society, (140): 9972-9978. 2018. 10.1021/jacs.8b05055

Xu, J. Z.; Yi, L. G.; Mou, Y. X.; Cao, J. P.; Wang, C. J.

Effect of a molecule of imidazolium bromide ionic liquid on the structure and properties of cytosine by density functional theory

Chemical Physics Letters, (708): 109-116. 2018. 10.1016/j.cplett.2018.08.009

Xu, M. F.; Zhang, B. H.; Wang, Q.; Yuan, Y.; Sun, L.; Huang, Z. G.

THEORETICAL STUDY ON THE HYDROGEN BONDING INTERACTIONS IN PARACETAMOL-WATER COMPLEXES

Journal of the Chilean Chemical Society, (63): 3788-3794. 2018. 10.4067/s0717-97072018000103788

Xu, Q. F.; Niu, Y. J.; Wang, G.; Li, Y. G.; Zhao, Y.; Singh, V.; Niu, J. Y.; Wang, J. P.

Polyoxoniobates as a superior Lewis base efficiently catalyzed Knoevenagel condensation  
Molecular Catalysis, (453): 93-99. 2018. 10.1016/j.mcat.2018.05.002

Xu, W. B.; Qiu, Y. L.; Zhang, T. T.; Li, X. F.; Zhang, H. M.

The Effect of Organic Additives on the Activity and Selectivity of CO<sub>2</sub> Electroreduction: The Role of Functional Groups

Chemsuschem, (11): 2904-2911. 2018. 10.1002/cssc.201801458

Xu, X. L.; Yang, B.; Wei, Z. Y.; Cao, G. J.; Xu, H. G.; Zheng, W. J.

Structural and bonding properties of Cu<sub>3</sub>O<sub>3</sub><sup>-</sup> and Cu<sub>3</sub>O<sub>4</sub><sup>-</sup> clusters: anion photoelectron spectroscopy and density functional calculations

Physical Chemistry Chemical Physics, (20): 20622-20628. 2018. 10.1039/c8cp03302a

Xu, Y.; Hua, E.  
Hydrogen Bonding Study on Protic Ionic Liquids Composed of N-Alkyl Ethylenediaminium Cations with Trifluoroacetic Anion  
Chemical Journal of Chinese Universities-Chinese, (39): 1954-1960. 2018. 10.7503/cjcu20180309

Xu, Z. X.; Zhao, Y. L.; Liang, W. Y.; Zhou, P. P.; Yang, Y.  
A novel N-methylimidazolium-based poly(ionic liquid) to recover trace tetrachloroaurate from aqueous solution based on multiple supramolecular interactions  
Inorganic Chemistry Frontiers, (5): 922-931. 2018. 10.1039/c7qi00753a

Yada, A.; Nagata, K.; Ando, Y.; Matsumura, T.; Ichinoseki, S.; Sato, K.  
Machine Learning Approach for Prediction of Reaction Yield with Simulated Catalyst Parameters  
Chemistry Letters, (47): 284-287. 2018. 10.1246/cl.171130

Yadav, A.; Lama, P.; Bienko, A.; Bienko, D.; Siddiqui, K. A.  
H-bonded supramolecular synthon induced magnetic superexchange phenomenon results weak ferromagnetic and strong antiferromagnetic interactions in two new copper-orotate coordination network  
Polyhedron, (141): 247-261. 2018. 10.1016/j.poly.2017.11.047

Yadav, S.; Goel, N.; Kumar, V.; Tikoo, K.; Singhal, S.  
Removal of fluoroquinolone from aqueous solution using graphene oxide: experimental and computational elucidation  
Environmental Science and Pollution Research, (25): 2942-2957. 2018. 10.1007/s11356-017-0596-8

Yadav, T.; Mukherjee, V.  
Interpretation of IR and Raman spectra of dopamine neurotransmitter and effect of hydrogen bond in HCl  
Journal of Molecular Structure, (1160): 256-270. 2018. 10.1016/j.molstruc.2018.01.066

Yadav, T.; Mukherjee, V.  
Structural confirmation and spectroscopic study of a biomolecule: Norepinephrine  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (202): 222-237. 2018. 10.1016/j.saa.2018.05.040

Yaghoobi, F.; Sohrabi-Mahboub, M.  
Theoretical Study on the Aza-Diels-Alder Reaction Catalyzed by PHCl<sub>2</sub> Lewis Acid via Pnicogen Bonding  
Journal of Physical Chemistry A, (122): 2781-2791. 2018. 10.1021/acs.jpca.7b12400

Yahia, W.; Nacereddine, A. K.; Liacha, M.; Djerourou, A.  
A quantum-chemical DFT study of the mechanism and regioselectivity of the 1,3-dipolar cycloaddition reaction of nitrile oxide with electron-rich ethylenes

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25540

Yahyaei, H.; Shahab, S.; Sheikhi, M.; Filippovich, L.; Almodarresiyeh, H. A.; Kumar, R.; Dikusar, E.; Borzehandani, M. Y.; Alnajjar, R.

Anisotropy (optical, electrical and thermal conductivity) in thin polarizing films for UV/Vis regions of spectrum: Experimental and theoretical investigations

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (192): 343-360. 2018. 10.1016/j.saa.2017.11.029

Yamada, A.; Yoshida, E.; Eda, K.; Osakai, T.

Prediction of the Standard Gibbs Energy of Ion Transfer across the 1,2-Dichloroethane/Water Interface

Analytical Sciences, (34): 919-924. 2018.

Yamane, M.; Yamashita, M.; Yamamoto, K.; Murahashi, T.

Contiguous multiple pi-coordination of pi-conjugated polyenes: bonding nature and charge delocalization behaviour of polyene-(palladium chain) sandwich clusters

Physical Chemistry Chemical Physics, (20): 4287-4296. 2018. 10.1039/c7cp06735f

Yan, C. X.; Yang, F.; Wu, R. Z.; Zhou, D. G.; Yang, X.; Zhou, P. P.

Application of Natural Orbital Fukui Functions and Bonding Reactivity Descriptor in Understanding Bond Formation Mechanisms Underlying 2+4 and 4+2 Cycloadditions of o-Thioquinones with 1,3-Dienes

Acta Physico-Chimica Sinica, (34): 497-502. 2018. 10.3866/pku.Whxb201709222

Yan, C. X.; Zhou, P. P.; Yang, F. L.; Wu, R. Z.; Yang, X.; Yang, F.; Shao, X. F.

Chiral bisoxazoline catalyzed decarboxylative aldol reactions between -carbonyl acids and trifluoroacetaldehyde hemiacetals as well as trifluoroacetaldehyde: the mechanism, the origin of enantioselectivity and the role of a catalyst

Organic Chemistry Frontiers, (5): 2692-2709. 2018. 10.1039/c8qo00578h

Yan, D.; Li, H. J.; Cai, H. Q.; Wang, M.; Wang, C. C.; Yi, H. B.; Min, X. B.

Microscopic insight into precipitation and adsorption of As(V) species by Fe-based materials in aqueous phase

Chemosphere, (194): 117-124. 2018. 10.1016/j.chemosphere.2017.11.150

Yan, H. M.; Tian, Y.; Li, N.; Chang, R.; Zhang, Z. X.; Zhang, X. Y.; Yang, W. J.; Guo, Z.; Li, Y. R.

Computational study on palladium-catalyzed alkenylation of remote delta-C(sp<sup>3</sup>)-H bonds with alkynes: a new understanding of mechanistic insight and origins of site-selectivity

RSC Advances, (8): 30186-30190. 2018. 10.1039/c8ra06077k

Yan, J.; Liu, C. B.; Zhang, D. J.

Theoretical insight into the mechanism, regioselectivity, and substituent group effect of Rh-catalyzed synthesis of 1,2-benzothiazines from NH-sulfoximines and diazo compounds

Organic & Biomolecular Chemistry, (16): 5321-5331. 2018. 10.1039/c8ob00996a

Yan, P. J.; Yao, X. Q.; Geng, Z. Y.; Wang, Q. Y.

Mechanistic insights into the chemoselectivity of PtCl<sub>n</sub> (n=2, 4)-catalyzed O-H insertion and cyclopropanation compared to Rh- and Cu-catalyzed reactions

Computational and Theoretical Chemistry, (1139): 55-62. 2018. 10.1016/j.comptc.2018.07.002

Yan, S. S.; Zhu, L.; Ye, J. H.; Zhang, Z.; Huang, H.; Zeng, H. Y.; Li, C. J.; Lan, Y.; Yu, D. G.

Ruthenium-catalyzed umpolung carboxylation of hydrazones with CO<sub>2</sub>

Chemical Science, (9): 4873-4878. 2018. 10.1039/c8sc01299g

Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N.

Dibromometallyl-iron complexes generated by the recombination of an alumanyl-iron complex with EBr<sub>3</sub> (E = Al, Ga)

Heteroatom Chemistry, (29) 2018. 10.1002/hc.21465

Yanai, H.; Almendros, P.; Takahashi, S.; Lazaro-Milla, C.; Alcaide, B.; Matsumoto, T.

Synthesis and Characterization of Stable Phosphorus Carbabetaaines

Chemistry-an Asian Journal, (13): 1956-1961. 2018. 10.1002/asia.201800769

Yang, B.; Xu, H. G.; Xu, X. L.; Zheng, W. J.

Photoelectron Spectroscopy and Theoretical Study of Cr<sub>n</sub>Si<sub>15-n</sub> (n=1-3): Effects of Doping Cr Atoms on the Structural and Magnetic Properties

Journal of Physical Chemistry A, (122): 9886-9893. 2018. 10.1021/acs.jpca.8b10588

Yang, C. Q.; Guo, W.; Lin, Y. L.; Lin, Q. Q.; Wang, J. J.; Wang, Y. L.

Experimental and DFT simulation study of a novel felodipine cocrystal: Characterization, dissolving properties and thermal decomposition kinetics

Journal of Pharmaceutical and Biomedical Analysis, (154): 198-206. 2018.

10.1016/j.jpba.2018.03.006

Yang, F.; Li, Y. X.; Dang, X.; Guo, H. J.; Chai, X. X.

Theoretical Study on the Transition State of N-nitropyrazoles Rearrangement Reaction

Chinese Journal of Structural Chemistry, (37): 531-542. 2018. 10.14102/j.cnki.0254-5861.2011-1765

Yang, F. L.; Lu, K.; Yang, X.; Yan, C. X.; Wang, R.; Ye, W. C.; Zhou, P. P.; Yang, Z. Y.

Computational investigations of intermolecular interactions between electron-accepting bromo- and iodo-pentafluorobenzene and electron-donating furan and thiophene

New Journal of Chemistry, (42): 20101-20112. 2018. 10.1039/c8nj04611e

Yang, F. L.; Yang, X.; Wu, R. Z.; Yan, C. X.; Yang, F.; Ye, W. C.; Zhang, L. W.; Zhou, P. P.

Intermolecular interactions between sigma- and pi-holes of bromopentafluorobenzene and pyridine: computational and experimental investigations

Physical Chemistry Chemical Physics, (20): 11386-11395. 2018. 10.1039/c8cp00420j

Yang, G. Y.; Wu, J.; Chen, S. G.; Zhou, W. J.; Sun, J.; Chen, G. H.

Size-independent neural networks based first-principles method for accurate prediction of heat of formation of fuels

Journal of Chemical Physics, (148) 2018. 10.1063/1.5024442

Yang, H.; Li, Y.; He, H. M.; Yu, D.; Wu, D.; Li, Z. R.

Hetero-binuclear superhalogen anions with cyanide and/or isocyanide as ligands

Chemical Physics Letters, (713): 203-209. 2018. 10.1016/j.cplett.2018.10.039

Yang, H.; Wu, D.; He, H. M.; Yu, D.; Li, Y.; Li, Z. R.

The behavior of the aluminum trimer when combining with different superatom clusters

RSC Advances, (8): 6667-6674. 2018. 10.1039/c7ra12852e

Yang, H. H.; Song, Y.; Zhang, Y.; Chen, H. S.

Prediction of the electron redundant  $\text{Si}_n\text{N}_n$  fullerenes

Physica E-Low-Dimensional Systems & Nanostructures, (99): 208-214. 2018.

10.1016/j.physe.2018.02.010

Yang, J.; Li, A. Y.

Hydrogen bond strengthening between o-nitroaniline and formaldehyde in electronic excited states: A theoretical study

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (199): 194-201. 2018.

10.1016/j.saa.2018.03.062

Yang, J. Q.; Gong, X. D.; Mei, H. Z.; Li, T.; Zhang, J. G.; Gozin, M.

Design of Zero Oxygen Balance Energetic Materials on the Basis of Diels-Alder Chemistry

Journal of Organic Chemistry, (83): 14698-14702. 2018. 10.1021/acs.joc.8b02000

Yang, J. Y.; Jiang, X. Y.; Jiao, F. P.; Yu, J. G.

The oxygen-rich pentaerythritol modified multi-walled carbon nanotube as an efficient adsorbent for aqueous removal of alizarin yellow R and alizarin red S

Applied Surface Science, (436): 198-206. 2018. 10.1016/j.apsusc.2017.12.029

Yang, M. X.; Pati, N.; Belanger-Chabot, G.; Hirai, M.; Gabbai, F. P.

Influence of the catalyst structure in the cycloaddition of isocyanates to oxiranes promoted by tetraarylstibonium cations

Dalton Transactions, (47): 11843-11850. 2018. 10.1039/c8dt00702k

Yang, M. X.; Tofan, D.; Chen, C. H.; Jack, K. M.; Gabbai, F. P.

Digging the Sigma-Hole of Organoantimony Lewis Acids by Oxidation

Angewandte Chemie-International Edition, (57): 13868-13872. 2018. 10.1002/anie.201808551

- Yang, P. Y.; Chen, H. Y.; Ju, S. P.; Chang, C. L.; Leu, G. S.; Lin, C. H.  
Catalytic polymerization of naphthalene by HF/BF<sub>3</sub> super acid: an ab initio density functional theory study  
Physical Chemistry Chemical Physics, (20): 23311-23319. 2018. 10.1039/c8cp02777c
- Yang, T.; Andrada, D. M.; Frenking, G.  
Dative versus electron-sharing bonding in N-oxides and phosphane oxides R<sub>3</sub>EO and relative energies of the R<sub>2</sub>EOR isomers (E = N, P; R = H, F, Cl, Me, Ph). A theoretical study  
Physical Chemistry Chemical Physics, (20): 11856-11866. 2018. 10.1039/c8cp00951a
- Yang, Y. S.; Yang, X.; Zhang, Y.; Xue, Y.  
Computational Mechanism Study on Allylic Oxidation of cis-Internal Alkenes: Insight into the Lewis Acid-Assisted Bronsted Acid (LBA) Catalysis in Heteroene Reactions  
Journal of Organic Chemistry, (83): 13344-13355. 2018. 10.1021/acs.joc.8b02130
- Yang, Y. Y.; Liu, Y. H.; Lv, P. L.; Zhu, R. X.; Liu, C. B.; Zhang, D. J.  
Theoretical Insight into the Mechanism and Origin of Ligand-Controlled Regioselectivity in Homogenous Gold-Catalyzed Intramolecular Hydroarylation of Alkynes  
Journal of Organic Chemistry, (83): 2763-2772. 2018. 10.1021/acs.joc.7b03213
- Yano, T.; Wasada-Tsutsui, Y.; Ikeda, T.; Shibayama, T.; Kajita, Y.; Inomata, T.; Funahashi, Y.; Ozawa, T.; Masuda, H.  
Co(III) Complexes with N<sub>2</sub>S<sub>3</sub>-Type Ligands as Structural/Functional Models for the Isocyanide Hydrolysis Reaction Catalyzed by Nitrile Hydratase  
Inorganic Chemistry, (57): 4277-4290. 2018. 10.1021/acs.inorgchem.6b02324
- Yao, H.; Minami, H.; Funada, T.  
Organic nanoparticles based on Lewis-pair formation: observation of prototypically controlled dual fluorescence  
Photochemical & Photobiological Sciences, (17): 1376-1385. 2018. 10.1039/c8pp00256h
- Yao, L. Y.; Li, Y.; Huang, L. T.; Guo, K.; Ren, G. R.; Wu, Z. Y.; Lei, Q. F.; Fang, W. J.; Xie, H. J.  
A DFT study on the mechanisms of hydrogenation and hydrosilylation of nitrous oxide catalyzed by a ruthenium PNP pincer complex  
Computational and Theoretical Chemistry, (1128): 48-55. 2018. 10.1016/j.comptc.2018.02.010
- Yao, Y. F.; Xu, Z.; Cheng, F.; Li, W. C.; Cui, P. X.; Xu, G. Z.; Xu, S.; Wang, P.; Sheng, G. D.; Yan, Y. D.; Yu, Z. T.; Yan, S. C.; Chen, Z. X.; Zou, Z. G.  
Unlocking the potential of graphene for water oxidation using an orbital hybridization strategy  
Energy & Environmental Science, (11): 407-416. 2018. 10.1039/c7ee02972a
- Yaremenko, I. A.; Gomes, G. D.; Radulov, P. S.; Belyakova, Y. Y.; Vilikotskiy, A. E.; Vil, V. A.; Korlyukov, A. A.; Nikishin, G. I.; Alabugin, I. V.; Terent'ev, A. O.

Ozone-Free Synthesis of Ozonides: Assembling Bicyclic Structures from 1,5-Diketones and Hydrogen Peroxide

Journal of Organic Chemistry, (83): 4402-4426. 2018. 10.1021/acs.joc.8b00130

Yasarawan, N.; Thipyapong, K.

Complexation reactions, electronic properties, and reactivity descriptors of cysteamine-based ligands in aqueous solution: a PCM/DFT study

Structural Chemistry, (29): 1723-1737. 2018. 10.1007/s11224-018-1151-z

Yavari, M.; Beyramabadi, S. A.; Morsali, A.; Bozorgmehr, M. R.

Tautomerization Reaction, Experimental and Theoretical Characterizations of the N,N-Dipyridoxyl(4-Methyl-1,2-Phenylenediamine) Schiff Base and its Cu(II) Complex

Journal of Structural Chemistry, (59): 1102-1113. 2018. 10.1134/s0022476618050128

Yi, J. C.; Fang, H.

Effect of different alkyl groups on excited-state tautomerization of 7Al-azaindole-H<sub>2</sub>O: A theoretical study

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (202): 58-64. 2018. 10.1016/j.saa.2018.05.037

Yi, J. C.; Fang, H.

Theoretical study on the substituent effect of halogen atom at different position of 7-azaindole-water derivatives: relative stability and excited-state proton-transfer mechanism

Structural Chemistry, (29): 1341-1350. 2018. 10.1007/s11224-018-1119-z

Yi, J. C.; Fang, H.

Theoretical Study on the Substituent Effect on the Excited-State Proton Transfer in the 7-Azaindole-Water Derivatives

Photochemistry and Photobiology, (94): 27-35. 2018. 10.1111/php.12839

Yi, S. F.; Wan, Y. L.; Wang, X. Y.

Interaction of beta-Cyclodextrin Catalyst with p-Chlorobenzonitrile for the Synthesis of 5-Substituted 1H-tetrazoles in n,n-Dimethylformamide: a DFT Study

Chinese Journal of Structural Chemistry, (37): 1523-1532. 2018. 10.14102/j.cnki.0254-5861.2011-1939

Yildirim, S. O.; Buyukmumcu, Z.; Dogan, S. D.; Butcher, R. J.

Redetermination and Density Functional Studies of N,N-(Disulfanediyldibenzene-2,1-Diyl) Dipyridine-2-Carboxamide

Journal of Structural Chemistry, (59): 1797-1803. 2018. 10.1134/s0022476618080061

Yildiz, C. B.

Oxidation of hydro-silaimine, phosphasilene, and arsilene structures (CH<sub>3</sub>)HSi=E(CH<sub>3</sub>) (E: N, P, or As) via concerted 1,3-dipolar cycloaddition of nitrous oxide: A DFT study

Computational and Theoretical Chemistry, (1134): 47-53. 2018. 10.1016/j.comptc.2018.05.003

Yin, J. L.; Zhou, F. L.; Zhu, L.; Yang, M. F.; Lan, Y.; You, J. S.

Annulation cascade of arylnitriles with alkynes to stable delocalized PAH carbocations via intramolecular rhodium migration

Chemical Science, (9): 5488-5493. 2018. 10.1039/c8sc01963k

Yin, S.; Bernstein, E. R.

Photoelectron spectroscopy and density functional theory studies of (FeS)(m)H- (m=2-4) cluster anions: effects of the single hydrogen

Physical Chemistry Chemical Physics, (20): 367-382. 2018. 10.1039/c7cp07012h

Yin, Y. Q.; Jiang, M. X.; Liu, C. G.

DFT Study of POM-Supported Single Atom Catalyst (M-1/POM, M = Ni, Pd, Pt, Cu, Ag, Au, POM = PW12O40 (3-)) for Activation of Nitrogen Molecules

Acta Physico-Chimica Sinica, (34): 270-277. 2018. 10.3866/pku.Whxb201707071

Yoosefian, M.

A high efficient nanostructured filter based on functionalized carbon nanotube to reduce the tobacco-specific nitrosamines, NNK

Applied Surface Science, (434): 134-141. 2018. 10.1016/j.apsusc.2017.10.166

Yoosefian, M.; Etminan, N.

Leucine/Pd-loaded (5,5) single-walled carbon nanotube matrix as a novel nanobiosensors for in silico detection of protein

Amino Acids, (50): 653-661. 2018. 10.1007/s00726-018-2552-4

Yoosefian, M.; Mola, A.; Hajiabadi, H.; Delouei, R. A.; Shahri, S. M. M.

Theoretical prediction of chloroform, ethanol, water and DMSO effects on electronic characteristics of Capecitabine different conformers as an anticancer chemotherapy drug

Journal of Molecular Liquids, (264): 115-118. 2018. 10.1016/j.molliq.2018.04.115

Yoosefian, M.; Pakpour, A.; Etminan, N.

Nanofilter platform based on functionalized carbon nanotubes for adsorption and elimination of Acrolein, a toxicant in cigarette smoke

Applied Surface Science, (444): 598-603. 2018. 10.1016/j.apsusc.2018.03.108

Yoosefian, M.; Rahmanifar, E.; Etminan, N.

Nanocarrier for levodopa Parkinson therapeutic drug; comprehensive benserazide analysis

Artificial Cells Nanomedicine and Biotechnology, (46): S434-S446. 2018.

10.1080/21691401.2018.1430583

You, D.; Yang, H. F.; Sen, S.; Gabbai, F. P.

Modulating the sigma-Accepting Properties of an Antimony Z-type Ligand via Anion Abstraction:  
Remote-Controlled Reactivity of the Coordinated Platinum Atom  
Journal of the American Chemical Society, (140): 9644-9651. 2018. 10.1021/jacs.8b05520

You, X. R.; Zhai, H. J.  
On the Nature of Bonding in Synthetic Charged Molecular Alloy P<sub>7</sub>ZnP<sub>7</sub> (4-) Cluster and Its  
Relevant P-7 (3-) Zintl Ion  
ACS Omega, (3): 11958-11965. 2018. 10.1021/acsomega.8b01790

Yu, D. H.; Du, R. B.; Xiao, J. C.; Xu, S. M.; Rong, C. Y.; Liu, S. B.  
Theoretical Study of pK(a) Values for Trivalent Rare-Earth Metal Cations in Aqueous Solution  
Journal of Physical Chemistry A, (122): 700-707. 2018. 10.1021/acs.jpca.7b12074

Yu, F.  
Dynamic exit-channel pathways of the microsolvated HOO-(H<sub>2</sub>O) + CH<sub>3</sub>Cl S(N)<sub>2</sub> reaction:  
Reaction mechanisms at the atomic level from direct chemical dynamics simulations  
Journal of Chemical Physics, (148) 2018. 10.1063/1.5000400

Yu, X. W.; Boyer, M. J.; Hwang, G. S.; Manthiram, A.  
Room-Temperature Aluminum-Sulfur Batteries with a Lithium-Ion-Mediated Ionic Liquid  
Electrolyte  
Chem, (4): 586-598. 2018. 10.1016/j.chempr.2017.12.029

Yu, Y.; Karayaylali, P.; Katayama, Y.; Giordano, L.; Gauthier, M.; Maglia, F.; Jung, R.; Lund, I.; Shao-Horn, Y.  
Coupled LiPF<sub>6</sub> Decomposition and Carbonate Dehydrogenation Enhanced by Highly Covalent  
Metal Oxides in High-Energy Li-Ion Batteries  
Journal of Physical Chemistry C, (122): 27368-27382. 2018. 10.1021/acs.jpcc.8b07848

Yu, Z.; Fang, C.; Huang, J. S.; Sumpter, B. G.; Qiao, R.  
Solvate Ionic Liquids at Electrified Interfaces  
ACS Applied Materials & Interfaces, (10): 32151-32161. 2018. 10.1021/acsami.8b10387

Yuan, B. F.; He, R. X.; Guo, X. G.; Shen, W.; Zhang, F. Y.; Xu, Y. Y.; Li, M.  
DFT study on the Au(I)-catalyzed cyclization of indole-allenoate: counterion and solvent effects  
New Journal of Chemistry, (42): 15618-15628. 2018. 10.1039/c8nj02375a

Yuan, H. Y.; Zhu, L. H.; Li, W. L.; Zhang, J. P.  
Mechanistic insight on water and substrate catalyzed the synthesis of 3-(1H-indol-3-yl)-2-(4-methoxybenzyl)isoindolin-1-one: Driving by noncovalent interactions  
Journal of Computational Chemistry, (39): 2316-2323. 2018. 10.1002/jcc.25563

Yuan, Q.; Toroz, D.; Kidley, N.; Gould, I. R.

Mechanism of Photoinduced Triplet Intermolecular Hydrogen Transfer between Cycloxydim and Chlorothalonil

Journal of Physical Chemistry A, (122): 4285-4293. 2018. 10.1021/acs.jpca.7b12523

Yuan, R. M.; Xu, S. H.; Fu, G.

Mechanisms of CO<sub>2</sub> Incorporation into Propargylic Amine Catalyzed by Ag(I)/Amine Catalysts  
Journal of Organic Chemistry, (83): 11896-11904. 2018. 10.1021/acs.joc.8b01767

Yuan, Y. N.; Wang, G. Y.; Zhang, X. X.; Nie, Y. X.; Geng, Z. Y.

A theoretical mechanistic study for C-H and C-C bond activations of cyclohexane catalyzed by NiAl+ in the gas phase

Computational and Theoretical Chemistry, (1129): 48-56. 2018. 10.1016/j.comptc.2018.02.015

Yuan, Y. N.; Xin, S. F.; Zhao, P. P.; Geng, Z. Y.

Theoretical investigation on cyclohexane dehydrogenation catalyzed by V-2(+) in gas-phase  
Structural Chemistry, (29): 1129-1137. 2018. 10.1007/s11224-018-1097-1

Zabardasti, A.; Farhadi, S.; Mahdizadeh, A.

Cooperative effect between pnictogen bond and hydrogen bond interactions in typical X horizontal ellipsis AsH<sub>2</sub>F horizontal ellipsis HF complexes (X = NR<sub>3</sub>, PR<sub>3</sub> and OR<sub>2</sub>; R = CH<sub>3</sub>, H, F)

Phosphorus Sulfur and Silicon and the Related Elements, (193): 759-765. 2018.

10.1080/10426507.2018.1513514

Zaboli, M.; Raissi, H.

A combined molecular dynamics simulation and quantum mechanics study on mercaptapurine interaction with the cucurbit 6,7 urils: Analysis of electronic structure

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (188): 647-658. 2018.

10.1016/j.saa.2017.07.058

Zacharias, A. O.; Varghese, A.; Akshaya, K. B.; Savitha, M. S.; George, L.

DFT, spectroscopic studies, NBO, NLO and Fukui functional analysis of 1-(1-(2,4-difluorophenyl)-2-(1H-1,2,4-triazol-1-yl)ethylidene) thiosemicarbazide

Journal of Molecular Structure, (1158): 1-13. 2018. 10.1016/j.molstruc.2018.01.002

Zahedi, M.; Shaabani, B.; Aygun, M.; Kazak, C.

Construction of one dimensional Co(II) and Zn( II) coordination polymers based on expanded N, N '-donor ligands

Inorganica Chimica Acta, (469): 461-468. 2018. 10.1016/j.ica.2017.09.023

Zahedi, M.; Shaabani, B.; Englert, U.; van Leusen, J.

Organic-inorganic hybrid materials from divalent metal cations and expanded N,N '-donor linkers

Zeitschrift Fur Kristallographie-Crystalline Materials, (233): 97-111. 2018. 10.1515/zkri-2017-2084

- Zaiter, A.; Zouchoune, B.  
Electronic structure and energy decomposition of binuclear transition metal complexes containing beta-diketiminate and imido ligands: spin state and metal's nature effects  
Structural Chemistry, (29): 1307-1320. 2018. 10.1007/s11224-018-1112-6
- Zakarianezhad, M.; Makiabadi, B.; Habibi-Khorassani, S. M.; Shool, M.; Eslamlou, M.  
Theoretical study on mechanism of reaction between tert-butyl isocyanide and dimethyl acetylenedicarboxylate in presence of ethanethiol or thiophenol  
Research on Chemical Intermediates, (44): 2653-2665. 2018. 10.1007/s11164-018-3252-0
- Zamani, A.; Ghiasi, R.; Sadjadi, M. S.; Yousefi, M.  
Theoretical Study of Substituent Effect in Aryl Group Migration in (para-C<sub>6</sub>H<sub>4</sub>X)Mn(CO)(5) Complexes  
Russian Journal of Inorganic Chemistry, (63): 906-910. 2018. 10.1134/s0036023618070240
- Zamani, M.; Delfani, A. M.; Jabbari, M.  
Scavenging performance and antioxidant activity of gamma-alumina nanoparticles towards DPPH free radical: Spectroscopic and DFT-D studies  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (201): 288-299. 2018. 10.1016/j.saa.2018.05.004
- Zanatta, G.; da Silva, M. B.; da Silva, J. J. A.; dos Santos, R. C. R.; Sales, F. A. M.; Gottfried, C.; Caetano, E. W. S.; Freire, V. N.  
First-generation antipsychotic haloperidol: optical absorption measurement and structural, electronic, and optical properties of its anhydrous monoclinic crystal by first-principle approaches  
New Journal of Chemistry, (42): 13629-13640. 2018. 10.1039/c8nj01548a
- Zauliczny, M.; Ordyszewska, A.; Pikies, J.; Grubba, R.  
Bonding in Phosphanylphosphinidene Complexes of Transition Metals and their Correlation with Structures, P-31 NMR Spectra, and Reactivities  
European Journal of Inorganic Chemistry: 3131-3141. 2018. 10.1002/ejic.201800270
- Zayed, M. A.; El-desawy, M.; Eladly, A. A.  
Experimental and theoretical spectroscopic studies in relation to molecular structure investigation of para chloro, para fluoro and para nitro maleanilinic acids  
Computational Biology and Chemistry, (76): 338-356. 2018.  
10.1016/j.compbiochem.2018.08.006
- Zdanovskaia, M. A.; Schwarz, C. E.; Habib, A. D.; Hill, N. J.; Esselman, B. J.  
Access to Computational Chemistry for Community Colleges via WebMO  
Journal of Chemical Education, (95): 1960-1965. 2018. 10.1021/acs.jchemed.8b00310
- Zeng, X.; Li, N.; Jiao, Q. J.

Carbon-free energetic materials: computational study on nitro-substituted BN-cage molecules with high heat of detonation and stability

RSC Advances, (8): 14654-14662. 2018. 10.1039/c7ra13476b

Zhang, B.; Zhao, J.; Zhao, Z. X.

Multiconfiguration time-dependent Hartree-Fock treatment of electron correlation in strong-field ionization of H<sub>2</sub> molecules

Acta Physica Sinica, (67) 2018. 10.7498/aps.67.20172701

Zhang, C. J.; Fan, F.; Wang, Z. M.; Song, J. S.; Li, C. S.; Mo, Y. R.

B-Heterocyclic Carbene Arising from Charge Shift: A Computational Verification

Chemistry-a European Journal, (24): 10216-10223. 2018. 10.1002/chem.201801620

Zhang, F. Y.; Xu, H. L.; Su, Z. M.

Redox-switchable structures and NLO property: Li-2 doped into the cavity of pyridine helix

Organic Electronics, (57): 68-73. 2018. 10.1016/j.orgel.2018.02.030

Zhang, G. Q.; Song, J. J.; Fu, L. S.; Tang, K. S.; Su, Y.; Chen, D. Z.

Understanding and modulating the high-energy properties of noble-gas hydrides from their long-bonding: an NBO/NRT investigation on HNgCO(+)/CS+/OSi+ and HNgCN/NC (Ng = He, Ar, Kr, Xe, Rn) molecules

Physical Chemistry Chemical Physics, (20): 10231-10239. 2018. 10.1039/c8cp00306h

Zhang, H.; Shang, Y.; Zhao, H.; Li, C. Y.; Wang, X.; Han, B. Z.; Li, Z. S.

Theoretical Study on the Grafting Reaction of Maleimide to Polyethylene in the UV Radiation Cross-Linking Process

Polymers, (10) 2018. 10.3390/polym10091044

Zhang, J.; Li, W.; Cheng, J.; Liu, Z.; Li, Q.

Cooperative effects between π-hole triel and π-hole chalcogen bonds

RSC Advances, (8): 26580-26588. 2018. 10.1039/c8ra04106g

Zhang, J.; Zhao, L. L.; Liu, Y. X.; Li, M. Y.; Li, G.; Meng, X. R.

Two luminescent transition-metal-organic frameworks with a predesigned ligand as highly sensitive and selective iron(III) sensors

New Journal of Chemistry, (42): 6839-6847. 2018. 10.1039/c8nj00656c

Zhang, J. P.; Wang, Y.; Ma, J. B.; Jin, L.; Liu, F. T.; Bai, F. Q.

Density functional theory investigation on iridium(iii) complexes for efficient blue electrophosphorescence

RSC Advances, (8): 19437-19448. 2018. 10.1039/c8ra02858c

Zhang, J. R.; Li, W. Z.; Cheng, J. B.; Liu, Z. B.; Li, Q. Z.

Cooperative effects between pi-hole triel and pi-hole chalcogen bonds

RSC Advances, (8): 26580-26588. 2018. 10.1039/c8ra04106g

Zhang, J. R.; Wei, Y. X.; Li, W. Z.; Cheng, J. B.; Li, Q. Z.

Triel-hydride triel bond between ZX<sub>3</sub> (Z = B and Al; X = H and Me) and THMe<sub>3</sub> (T = Si, Ge and Sn)

Applied Organometallic Chemistry, (32) 2018. 10.1002/aoc.4367

Zhang, J. X.; Hubner, E. G.; Namyslo, J. C.; Nieger, M.; Schmidt, A.

Purine-substituted imidazolium mesomeric betaines and their tautomeric N-heterocyclic carbenes. Formation of a cyclic borane adduct

Organic & Biomolecular Chemistry, (16): 6801-6808. 2018. 10.1039/c8ob01916a

Zhang, J. X.; Sheong, F. K.; Lin, Z. Y.

Unravelling Chemical Interactions with Principal Interacting Orbital Analysis

Chemistry-a European Journal, (24): 9639-9650. 2018. 10.1002/chem.201801220

Zhang, K.; Noble, B. B.; Mater, A. C.; Monteiro, M. J.; Coote, M. L.; Jia, Z. F.

Effect of heteroatom and functionality substitution on the oxidation potential of cyclic nitroxide radicals: role of electrostatics in electrochemistry

Physical Chemistry Chemical Physics, (20): 2606-2614. 2018. 10.1039/c7cp07444a

Zhang, L.; Yu, L.; Zhou, J. G.; Chen, Y.

Meta-Selective C-H Alkylation of 2-Phenylpyridine Catalyzed by Ruthenium: DFT Study on the Mechanism and Regioselectivity

European Journal of Organic Chemistry: 5268-5277. 2018. 10.1002/ejoc.201800772

Zhang, L. F.; Meng, J. L.; Yao, F.; Liu, X. J.; Meng, J.; Zhang, H. J.

Strong-correlated behavior of 4f electrons and 4f5d hybridization in PrO<sub>2</sub>

Scientific Reports, (8) 2018. 10.1038/s41598-018-34336-4

Zhang, L. H.; Xia, X. X.; Sun, W. G.; Lu, C.; Kuang, X. Y.; Le Chen, B.; Maroulis, G.

Probing the Structural and Electronic Properties of Dirhenium Halide Clusters: A Density Functional Theory Study

Scientific Reports, (8) 2018. 10.1038/s41598-018-25027-1

Zhang, L. J.; Qie, M. Y.; Su, J.; Zhang, S.; Zhou, J.; Li, J.; Wang, Y.; Yang, S. T.; Wang, S. A.; Li, J. Y.; Wu, G. Z.; Wang, J. Q.

Tris-amidoximate uranyl complexes via eta(2) binding mode coordinated in aqueous solution shown by X-ray absorption spectroscopy and density functional theory methods

Journal of Synchrotron Radiation, (25): 514-522. 2018. 10.1107/s160057751800067x

Zhang, L. L.; Wang, X. Y.; Jiang, K. Y.; Zhao, B. Y.; Yan, H. M.; Zhang, X. Y.; Zhang, Z. X.; Guo, Z.; Che, C. M.

A theoretical study on the oxidation of alkenes to aldehydes catalyzed by ruthenium porphyrins using O<sub>2</sub> as the sole oxidant

Dalton Transactions, (47): 5286-5297. 2018. 10.1039/c8dt00614h

Zhang, N.; Dong, B. L.; Kong, X. Q.; Wang, C.; Song, W. H.; Lin, W. Y.

Development of a Xanthene-Based Red-Emissive Fluorescent Probe for Visualizing H<sub>2</sub>O<sub>2</sub> in Living Cells, Tissues and Animals

Journal of Fluorescence, (28): 681-687. 2018. 10.1007/s10895-018-2231-6

Zhang, S. W.; Adrian, L.; Schuurmann, G.

Interaction Mode and Regioselectivity in Vitamin B-12-Dependent Dehalogenation of Aryl Halides by Dehalococcoides mccartyi Strain CBDB1

Environmental Science & Technology, (52): 1834-1843. 2018. 10.1021/acs.est.7b04278

Zhang, T. L.; Lan, X. G.; Wang, R.; Roy, S.; Qiao, Z. Y.; Lu, Y. S.; Wang, Z. Q.

The catalytic effects of H<sub>2</sub>CO<sub>3</sub>, CH<sub>3</sub>COOH, HCOOH and H<sub>2</sub>O on the addition reaction of CH<sub>2</sub>OO + H<sub>2</sub>O -> CH<sub>2</sub>(OH)OOH

Molecular Physics, (116): 1783-1794. 2018. 10.1080/00268976.2018.1454612

Zhang, T. L.; Lan, X. G.; Wen, M. J.; Zhang, Y. Q.; Wang, R.; Wang, Z. Y.

Catalytic effect of water, water dimer, HCOOH and H<sub>2</sub>SO<sub>4</sub> on the isomerisation of HON(O)NNO<sub>2</sub> to ON(OH)NNO<sub>2</sub>: a mechanism study

Molecular Simulation, (44): 1544-1553. 2018. 10.1080/08927022.2018.1518578

Zhang, X. X.; Barraza, K. M.; Beauchamp, J. L.

Cholesterol provides nonsacrificial protection of membrane lipids from chemical damage at air-water interface

Proceedings of the National Academy of Sciences of the United States of America, (115): 3255-3260. 2018. 10.1073/pnas.1722323115

Zhang, X. X.; Lundell, K. A.; Olson, J. K.; Bowen, K. H.; Boldyrev, A. I.

Electronic Transmutation (ET): Chemically Turning One Element into Another  
Chemistry-a European Journal, (24): 9200-9210. 2018. 10.1002/chem.201800517

Zhang, Y.; Yang, Y. S.; Zhao, J. M.; Xue, Y.

Mechanism and Diastereoselectivity of 3+3 Cycloaddition between Enol Diazoacetate and Azomethine Imine Catalyzed by Dirhodium Tetracarboxylate: A Theoretical Study

European Journal of Organic Chemistry: 3086-3094. 2018. 10.1002/ejoc.201800261

Zhang, Y. J.; Liu, J. R.; Liu, L.; Zhang, X. H.; Li, Q. S.; King, R. B.

Binuclear vanadium dimethylphosphino carbonyls: vanadium-vanadium multiple bonds and four-electron donor carbonyl groups as structural features in unsaturated systems

Inorganica Chimica Acta, (476): 61-67. 2018. 10.1016/j.ica.2018.02.008

Zhang, Y. W.; Wang, Y. C.; Zhang, X. J.; Wang, X. L.; Li, S.

A theoretical study on La-activated bicyclo-oligomerization of acetylene to form naphthalene in gas phase using density functional theory (DFT)

Structural Chemistry, (29): 171-178. 2018. 10.1007/s11224-017-1016-x

Zhang, Z. F.; Ma, N. N.

A scarce C=C center dot center dot center dot C equivalent to N pi-hole interaction in (E)-isomers of 3- (4-halogenphenyl)amino -2-cyanoprop-2-enoates

New Journal of Chemistry, (42): 19995-20000. 2018. 10.1039/c8nj04000a

Zhao, D. X.; Zhao, J.; Zhu, Z. W.; Zhang, C.; Yang, Z. Z.

A model of atoms in molecules based on potential acting on one electron in a molecule: I. Partition and atomic charges obtained from ab initio calculations

International Journal of Quantum Chemistry, (118) 2018. 10.1002/qua.25610

Zhao, H. B.; Gui, J. F.; Cao, J.; Zheng, C. H.

Molecular Dynamics Simulation of the Microscopic Sintering Process of CuO Nanograins Inside an Oxygen Carrier Particle

Journal of Physical Chemistry C, (122): 25595-25605. 2018. 10.1021/acs.jpcc.8b04253

Zhao, J.; Beckers, H.; Huang, T. F.; Wang, X. F.; Riedel, S.

H<sub>2</sub>MBH<sub>2</sub> and M(mu-H)(2)BH<sub>2</sub> Molecules Isolated in Solid Argon: Interelement M-B and M-H-B Bonds (M = Ge, Sn)

Inorganic Chemistry, (57): 2218-2227. 2018. 10.1021/acs.inorgchem.7b03109

Zhao, K.; Song, J.; Zhu, M. Y.; Zhang, H.; Wang, C. K.

Isomerism and coordination mode effects on two-photon absorption of tris(picollyl)amine-based fluorescent probes for zinc ions

Chinese Physics B, (27) 2018. 10.1088/1674-1056/27/10/103301

Zhao, L. J.; Xu, X. L.; Xu, H. G.; Feng, G.; Zheng, W. J.

Structural and bonding properties of BS-/0 and BS<sub>3</sub>-/0

New Journal of Chemistry, (42): 16021-16026. 2018. 10.1039/c8nj01835a

Zhao, P. P.; Wang, Y. C.; Jia, Y. M.; Sheng, Y.

Theoretical investigation on the gas phase decomposition of ethyl acetate by Ni<sup>+</sup>  
Structural Chemistry, (29): 1449-1456. 2018. 10.1007/s11224-018-1125-1

Zhao, Q.; Kulik, H. J.

Electronic Structure Origins of Surface-Dependent Growth in III-V Quantum Dots  
Chemistry of Materials, (30): 7154-7165. 2018. 10.1021/acs.chemmater.8b03125

Zhao, R. F.; Zhou, F. Q.; Xu, W. H.; Li, J. F.; Li, C. C.; Li, J. L.; Yin, B.

Superhalogen-based composite with strong acidity-a crossing point between two topics  
Inorganic Chemistry Frontiers, (5): 2934-2947. 2018. 10.1039/c8qi00647d

Zhao, S. B.; Gensch, T.; Murray, B.; Niemeyer, Z. L.; Sigman, M. S.; Biscoe, M. R.  
Enantiodivergent Pd-catalyzed C-C bond formation enabled through ligand parameterization  
Science, (362): 670-. 2018. 10.1126/science.aat2299

Zhao, X. F.; Bian, J. H.; Huang, F.; Yuan, C. X.; Wang, Q.; Liu, P.; Li, D. B.; Wang, X. T.; Wu, Y. B.  
Stabilization of beryllium-containing planar pentacoordinate carbon species through attaching  
hydrogen atoms  
RSC Advances, (8): 36521-36526. 2018. 10.1039/c8ra07664b

Zhao, X. F.; Li, J. J.; Li, H. R.; Yuan, C. X.; Tian, X. X.; Li, S. D.; Wu, Y. B.; Guo, J. C.; Wang, Z. X.  
Viable aromatic BenHn stars enclosing a planar hypercoordinate boron or late transition metal  
Physical Chemistry Chemical Physics, (20): 7217-7222. 2018. 10.1039/c7cp06955c

Zhao, X. F.; Yuan, C. X.; Li, S. D.; Wu, Y. B.; Wang, X. T.  
Simulating the effect of a triple bond to achieve the shortest main group metal-metal distance in  
diberyllium complexes: a computational study  
Dalton Transactions, (47): 14462-14467. 2018. 10.1039/c8dt02683a

Zhao, Y.; Wang, W. H.; Feng, W. L.; Wang, W. L.; Li, P.  
Theoretical Insights into the Interaction Mechanisms between Nitric Acid and Nitrous Oxide  
Initiated by an Excess Electron  
Journal of Physical Chemistry A, (122): 7312-7319. 2018. 10.1021/acs.jpca.8b04775

Zhen, J. P.; Wei, X. C.; Shi, W. J.; Huang, Z. Y.; Jin, B.; Zhou, Y. K.  
Cooperativity effect involving drug-DNA/RNA intermolecular interaction: A B3LYP-D3 and MP2  
theoretical investigation on ketoprofen center dot center dot center dot cytosine center dot center dot  
center dot H2O system  
Journal of Biomolecular Structure & Dynamics, (36): 3587-3606. 2018.  
10.1080/07391102.2017.1400469

Zheng, B. S.; Liu, Y.; Huang, L.; Wang, Z. X.; Liu, H. X.; Liu, Y.  
Cooperative effects between F... Ag bonded and X ... Br (Cl) halogen-bonded interaction in  
BrF(CIF) ... AgX ... BrF(CIF) (X=F, Cl, Br) complexes: a theoretical study  
Molecular Physics, (116): 1834-1843. 2018. 10.1080/00268976.2018.1459001

Zheng, D.; Yuan, X. A.; Ma, H. B.; Li, X. X.; Wang, X. Z.; Liu, Z. T.; Ma, J.  
Unexpected solvent effects on the UV/Vis absorption spectra of o-cresol in toluene and  
benzene: in contrast with non-aromatic solvents  
Royal Society Open Science, (5) 2018. 10.1098/rsos.171928

Zheng, X. J.; Zhang, Y.; Cao, N.; Li, X.; Zhang, S. Q.; Du, R. F.; Wang, H. Y.; Ye, Z. N.; Wang, Y.; Cao, F. H.; Li,  
H. R.; Hong, X.; Sue, A. C. H.; Yang, C. L.; Liu, W. G.; Li, H.  
Coulombic-enhanced hetero radical pairing interactions

Nature Communications, (9) 2018. 10.1038/s41467-018-04335-0

Zheng, Y. P.; Li, H. H.; Yuan, H. Y.; Fan, H. H.; Li, W. L.; Zhang, J. P.

Understanding the anchoring effect of Graphene, BN, C<sub>2</sub>N and C<sub>3</sub>N<sub>4</sub> monolayers for lithium-polysulfides in Li-S batteries

Applied Surface Science, (434): 596-603. 2018. 10.1016/j.apsusc.2017.10.230

Zheng, Y. Y.; Zheng, W. R.; Wang, J. Y.; Chang, H. F.; Zhu, D. F.

Computational Study on N-N Homolytic Bond Dissociation Enthalpies of Hydrazine Derivatives  
Journal of Physical Chemistry A, (122): 2764-2780. 2018. 10.1021/acs.jpca.7b12094

Zhiani, R.; Razavipanah, I.; Emrani, S.

Functionalized single-walled carbon nanotube for ketamine sensing: DFT and MD studies  
Structural Chemistry, (29): 1807-1815. 2018. 10.1007/s11224-018-1160-y

Zhigulin, G. Y.; Zabrodina, G. S.; Katkova, M. A.; Ketkov, S. Y.

Quantum chemical study of formation of Cu-II-Y-III metallamacrocyclic complexes based on glycinehydroximate ligands

Russian Chemical Bulletin, (67): 1173-1181. 2018. 10.1007/s11172-018-2198-0

Zhong, A. G.; Li, R. R.; Hong, Q.; Zhang, J.; Chen, D.

Understanding the Isomerization of Monosubstituted Alkanes from Energetic and Information-Theoretic Perspectives

Acta Physico-Chimica Sinica, (34): 303-313. 2018. 10.3866/pku.Whxb201708302

Zhong, W. H.; Liu, Y. X.; Deng, M. S.; Zhang, Y. C.; Jia, C. Y.; Prezhdo, O. V.; Yuan, J. Y.; Jiang, J.

C<sub>2</sub>N-supported single metal ion catalysts for HCOOH dehydrogenation

Journal of Materials Chemistry A, (6): 11105-11112. 2018. 10.1039/c8ta02299b

Zhou, D.; Li, G. L.; Moore, K. B.; Xie, Y. M.; Peterson, K. A.; Schaefer, H. F.

Noncovalent Interactions between Molecular Hydrogen and the Alkali Fluorides: H-H center dot center dot center dot F-M (M = Li, Na, K, Rb, Cs). High Level Theoretical Predictions and SAPT Analysis

Journal of Chemical Theory and Computation, (14): 5118-5127. 2018. 10.1021/acs.jctc.8b00461

Zhou, F.; Zhang, J. S.; Fu, T. Y.; Bai, P.; Bai, P.; Guo, X. H.

Theoretical study on complexes and reactions of boron isotopic exchange separation with fluorinated anisoles as novel donors

Journal of Radioanalytical and Nuclear Chemistry, (316): 587-594. 2018. 10.1007/s10967-018-5824-2

Zhou, Q. H.; Tang, W. J.; Chung, L. W.

Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations

Journal of Organometallic Chemistry, (864): 97-104. 2018. 10.1016/j.jorgancem.2018.02.001

Zhou, X. X.; Li, Y. L.; Shao, Y. F.; Hua, Y. H.; Zhang, H.; Lin, Y. M.; Xia, H. P.

Reactions of Cyclic Osmacarbyne with Coinage Metal Complexes

Organometallics, (37): 1788-1794. 2018. 10.1021/acs.organomet.8b00214

Zhou, X. X.; Wu, J. J.; Hao, Y. L.; Zhu, C. Q.; Zhuo, Q. D.; Xia, H. P.; Zhu, J.

Rational Design and Synthesis of Unsaturated Se-Containing Osmacycles with sigma-Aromaticity

Chemistry-a European Journal, (24): 2389-2395. 2018. 10.1002/chem.201703870

Zhou, Z.; Spisak, S. N.; Xu, Q.; Rogachev, A. Y.; Wei, Z.; Marcaccio, M.; Petrukhina, M. A.

Fusing a Planar Group to a pi-Bowl: Electronic and Molecular Structure, Aromaticity and Solid-State Packing of Naphthocorannulene and its Anions

Chemistry-a European Journal, (24): 3455-3463. 2018. 10.1002/chem.201705814

Zhu, C.; Wang, Q.; Yun, J. N.; Hu, Q. L.; Yang, G.

Non-covalent interactions for carbonaceous materials: impacts of doping, curving and their combination

Physical Chemistry Chemical Physics, (20): 22228-22240. 2018. 10.1039/c8cp02286k

Zhu, C.; Yun, J. N.; Wang, Q.; Yang, G.

Adsorption of ion pairs onto graphene flakes and impacts of counterions during the adsorption processes

Applied Surface Science, (435): 329-337. 2018. 10.1016/j.apsusc.2017.11.105

Zhu, F.; Rodriguez, J.; O'Neill, S.; Walczak, M. A.

Acyl Glycosides through Stereospecific Glycosyl Cross-Coupling: Rapid Access to C(sp<sup>3</sup>))-Linked Glycomimetics

Acs Central Science, (4): 1652-1662. 2018. 10.1021/acscentsci.8b00628

Zhu, J. W.; Zins, E. L.; Alikhani, M. E.

Dehydrocoupling of dimethylamine borane by titanocene: elucidation of ten years of inconsistency between theoretical and experimental descriptions

Physical Chemistry Chemical Physics, (20): 15687-15695. 2018. 10.1039/c8cp01970c

Zhu, L. H.; Yuan, H. Y.; Li, W. L.; Zhang, J. P.

A computational mechanistic study of substrate-controlled competitive O-H and C-H insertion reactions catalyzed by dirhodium(II) carbenoids: insight into the origin of chemoselectivity

Organic Chemistry Frontiers, (5): 2353-2363. 2018. 10.1039/c8qo00475g

Zhu, T. Y.; de Silva, P.; Van Voorhis, T.

Self-Attractive Hartree Decomposition: Partitioning Electron Density into Smooth Localized Fragments

Journal of Chemical Theory and Computation, (14): 92-103. 2018. 10.1021/acs.jctc.7b00931

- Zhu, X.; Zhou, X. Q.; Xiang, D. S.; Wu, P.  
A theoretical study towards thermolysis process of thionesters and thioesters  
Journal of Theoretical & Computational Chemistry, (17) 2018. 10.1142/s0219633618500141
- Zhu, Y. Q.; Wang, Y.; Liu, X.; Mo, X. C.  
Au(I) and Au(III)-Catalyzed Mechanism of the Cyclization Reaction of 3-(Ethynylamino)-1,3-diphenylprop-2-en-1-one  
Russian Journal of Physical Chemistry A, (92): 1893-1899. 2018. 10.1134/s0036024418100394
- Zhu, Y. T.; Han, Z.; Fu, L. J.; Liu, C. B.; Zhang, D. J.  
Cleavage of the -O-4 bond in a lignin model compound using the acidic ionic liquid 1-H-3-methylimidazolium chloride as catalyst: a DFT mechanistic study  
Journal of Molecular Modeling, (24) 2018. 10.1007/s00894-018-3854-x
- Zierkiewicz, W.; Fanfrlik, J.; Michalczyk, M.; Michalska, D.; Hobza, P.  
S center dot center dot center dot N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study  
Chemical Physics, (500): 37-44. 2018. 10.1016/j.chemphys.2017.11.014
- Zierkiewicz, W.; Michalczyk, M.; Scheiner, S.  
Aerogen bonds formed between AeOF(2) (Ae = Kr, Xe) and diazines: comparisons between sigma-hole and pi-hole complexes  
Physical Chemistry Chemical Physics, (20): 4676-4687. 2018. 10.1039/c7cp08048d
- Zierkiewicz, W.; Michalczyk, M.; Scheiner, S.  
Comparison between Tetrel Bonded Complexes Stabilized by sigma and pi Hole Interactions  
Molecules, (23) 2018. 10.3390/molecules23061416
- Zierkiewicz, W.; Michalczyk, M.; Scheiner, S.  
Regium bonds between Mn clusters ( M = Cu, Ag, Au and n=2-6) and nucleophiles NH<sub>3</sub> and HCN  
Physical Chemistry Chemical Physics, (20): 22498-22509. 2018. 10.1039/c8cp03883j
- Zilberg, S.; Sivan, J.  
Triple BB bond: from a perfect Lewis structure to a dominant -back-donation. The need for a reference point  
Journal of Coordination Chemistry, (71): 2053-2064. 2018. 10.1080/00958972.2018.1490728
- Zimnicka, M. M.  
Conformational Features of Thioamide-Containing Dipeptoids and Peptoid-Peptide Hybrids-Computational and Experimental Approaches  
Journal of Physical Chemistry A, (122): 7819-7831. 2018. 10.1021/acs.jpca.8b05456
- Zobeydi, R.; Setayesh, S. R.

Theoretical studies of the influence of protic and aprotic ionic liquids on the basicity of CaO as a solid base catalyst

Chemical Physics, (504): 31-37. 2018. 10.1016/j.chemphys.2018.02.019

Zolfigol, M. A.; Khazaei, A.; Karimitabar, F.; Hamidi, M.; Maleki, F.; Aghabarari, B.; Sefat, F.; Mozafari, M.  
Synthesis of Indolo 3,2-b carbazoles via an Anomeric-Based Oxidation Process: A Combined Experimental and Computational Strategy

Journal of Heterocyclic Chemistry, (55): 1061-1068. 2018. 10.1002/jhet.3077

Zoller, T.; Dietz, C.; Winter, F.; Pottgen, R.; Gorelsky, S. I.; Hoffmann, A.; Herres-Pawlis, S.; Jurkschat, K.  
Rational Syntheses and Serendipity: Complexes  $\text{LSnPtCl}_2(\text{SMe}_2)_2$ ,  $\{\text{LSnPtCl}(\text{SMe}_2)\}_2\text{SnCl}_2$ ,  $(\text{LSn})_3(\text{PtCl}_2)(\text{PtCl}_2\text{SnCl})\{\text{LSn}(\text{Cl})\text{OH}\}$ , and  $\text{O}(\text{SnCl})_2(\text{SnL})_2$  with L = MeN(CH<sub>2</sub>CMe<sub>2</sub>O)<sub>2</sub>  
Chemistry-a European Journal, (24): 5551-5561. 2018. 10.1002/chem.201703520

Zorbaz, T.; Malinak, D.; Marakovic, N.; Hrvat, N. M.; Zandona, A.; Novotny, M.; Skarka, A.; Andrys, R.; Benkova, M.; Soukup, O.; Katalinic, M.; Kuca, K.; Kovarik, Z.; Musilek, K.  
Pyridinium Oximes with Ortho-Positioned Chlorine Moiety Exhibit Improved Physicochemical Properties and Efficient Reactivation of Human Acetylcholinesterase Inhibited by Several Nerve Agents  
Journal of Medicinal Chemistry, (61): 10753-10766. 2018. 10.1021/acs.jmedchem.8b01398

Zou, W. L.; Cai, Z. Y.; Wang, J. K.; Xin, K. Y.

An open library of relativistic core electron density function for the QTAIM analysis with pseudopotentials

Journal of Computational Chemistry, (39): 1697-1706. 2018. 10.1002/jcc.25214

Zou, W. L.; Zhang, X. L.; Dai, H. M.; Yan, H.; Cremer, D.; Kraka, E.

Description of an unusual hydrogen bond between carborane and a phenyl group

Journal of Organometallic Chemistry, (865): 114-127. 2018. 10.1016/j.jorgchem.2018.02.014

Zouchoune, B.

Stability and possible multiple metal-metal bonding in tetrานuclear sandwich complexes of cyclooctatetraene ligand

Structural Chemistry, (29): 937-945. 2018. 10.1007/s11224-018-1077-5

Zouchoune, B.; Saiad, A.

Ligands' sigma-donation and pi-backdonation effects on metal-metal bonding in trinuclear M-3(Tr)(2)(L)(3) (2+) (M = Fe, Ni, Pd, Pt, Tr = tropylium and L = CO, HCN and C<sub>2</sub>H<sub>4</sub>) sandwich compounds: Theoretical investigation

Inorganica Chimica Acta, (473): 204-215. 2018. 10.1016/j.ica.2018.01.004

Zouchoune, B.; Zendaoui, S. M.; Saillard, J. Y.

Why is bis-indenylchromium a dimer? A DFT investigation

Journal of Organometallic Chemistry, (858): 47-52. 2018. 10.1016/j.jorgchem.2017.12.035

Zulfikaroglu, A.; Bati, H.; Dege, N.

A theoretical and experimental study on isonitrosoacetophenone nicotinoyl hydrazone: Crystal structure, spectroscopic properties, NBO, NPA and NLMO analyses and the investigation of interaction with some transition metals

Journal of Molecular Structure, (1162): 125-139. 2018. 10.1016/j.molstruc.2018.02.079

Zuniga-Nunez, D.; Barrias, P.; Cardenas-Jiron, G.; Ureta-Zanartu, M. S.; Lopez-Alarcon, C.; Vieyra, F. E. M.; Borsarelli, C. D.; Alarcon, E. I.; Aspee, A.

Atypical antioxidant activity of non-phenolic amino-coumarins

RSC Advances, (8): 1927-1933. 2018. 10.1039/c7ra12000a

Zuo, Y. N.; Yang, N.; Huang, X. K.; Hu, C. W.; Su, Z. S.

Mechanism and Origins of Stereoinduction in an Asymmetric Friedel-Crafts Alkylation Reaction of Chalcone Catalyzed by Chiral N,N'-Dioxide-Sc(III) Complex

Journal of Organic Chemistry, (83): 4628-4640. 2018. 10.1021/acs.joc.8b00387