

NBO 2016 – 2008 references
Compiled by Ariel Andrea on 8/31/2018

- Aal, S. A.
Reactivity of boron- and nitrogen-doped carbon nanotubes functionalized by (Pt, Eu) atoms toward O-2 and CO: A density functional study
International Journal of Modern Physics C, (27) 2016. 10.1142/s0129183116500753
- Abbat, S.; Bharatam, P. V.
Electronic structure and conformational analysis of P218: An antimalarial drug candidate
International Journal of Quantum Chemistry, (116): 1362-1369. 2016. 10.1002/qua.25189
- Abbensem, J.; Finger, M.; Wurtele, C.; Kasanmascheff, M.; Schneider, S.
Coupling of terminal iridium nitrido complexes
Inorganic Chemistry Frontiers, (3): 469-477. 2016. 10.1039/c5qi00267b
- Abboud, J. L. M.; Alkorta, I.; Davalos, J. Z.; Koppel, I. A.; Koppel, I.; Lenoir, D.; Martinez, S.; Mishima, M.
The Thermodynamic Stability of Adamantylideneadamantane and Its Proton- and Electron-Exchanges. Comparison with Simple Alkenes
Bulletin of the Chemical Society of Japan, (89): 762-769. 2016. 10.1246/bcsj.20160026
- Abdalrazaq, S. M.; Cabir, B.; Gumus, S.; Agirtas, M. S.
Synthesis of metallophthalocyanines with four oxy-2,2-diphenylacetic acid substituents and their structural and electronic properties
Heterocyclic Communications, (22): 275-280. 2016. 10.1515/hc-2016-0120
- Abdelmoula, H.; Ghalla, H.; Nasr, S.; Bahri, M.; Bellissent-Funel, M. C.
Hydrogen-bond network in liquid ethylene glycol as studied by neutron scattering and DFT calculations
Journal of Molecular Liquids, (220): 527-539. 2016. 10.1016/j.molliq.2016.04.111
- Abdelmoula, H.; Ghalla, H.; Nasr, S.; Darpentigny, J.; Bellissent-Funel, M. C.
Intermolecular associations in an equimolar formamide-water solution based on neutron scattering and DFT calculations
Journal of Chemical Physics, (145) 2016. 10.1063/1.4963915
- Abdullah, H. Y.
Theoretical study of the binding energy of some gases on Al-doped carbon nanotube
Results in Physics, (6): 1146-1151. 2016. 10.1016/j.rinp.2016.11.053
- Abdulsattar, M. A.
Electronic and spectroscopic properties of Ge nanocrystals using diamondoid structures: A density functional theory study
International Journal of Modern Physics B, (30) 2016. 10.1142/s0217979216500582
- Abdulsattar, M. A.; Abduljalil, H. M.; Al-Aaraji, N.
Spectroscopic Properties of AlSb Nanocrystals Using Diamondoid Structures: A Density Functional Theory Study
Nanomaterials and Nanotechnology, (6) 2016. 10.5772/62197
- Abelard, J.; Wilmsmeyer, A. R.; Edwards, A. C.; Gordon, W. O.; Durke, E. M.; Karwacki, C. J.; Troya, D.; Morris, J. R.
Adsorption of Substituted Benzene Derivatives on Silica: Effects of Electron Withdrawing and Donating Groups
Journal of Physical Chemistry C, (120): 13024-13031. 2016. 10.1021/acs.jpcc.6b02028
- Ablat, H.; Povey, I.; O'Kane, R.; Cahill, S.; Elliott, S. D.
The role of local chemical hardness and van der Waals interactions in the anionic polymerization of alkyl cyanoacrylates
Polymer Chemistry, (7): 3236-3243. 2016. 10.1039/c6py00201c
- Aboelnaga, A.; Hagar, M.; Soliman, S. M.

Ultrasonic Synthesis, Molecular Structure and Mechanistic Study of 1,3-Dipolar Cycloaddition Reaction of 1-Alkynylpyridinium-3-olate and Acetylene Derivatives
Molecules, (21) 2016. 10.3390/molecules21070848

Abroshan, H.; Dhumal, N. R.; Shim, Y.; Kim, H. J.
Theoretical study of interactions of a Li⁺(CF₃SO₂)₂N- ion pair with CR₃(OCR₂CR₂)(n)OCR₃ (R = H or F)
Physical Chemistry Chemical Physics, (18): 6754-6762. 2016. 10.1039/c6cp00139d

Acosta-Silva, C.; Bertran, J.; Branchadell, V.; Oliva, A.
Theoretical Insights on the Mechanism of the GTP Hydrolysis Catalyzed by the Elongation Factor Tu (EF-Tu)
Journal of Physical Chemistry B, (120): 89-101. 2016. 10.1021/acs.jpcb.5b10145

Adasme-Carreno, F.; Munoz-Gutierrez, C.; Alzate-Morales, J. H.
Halogen bonding in drug-like molecules: a computational and systematic study of the substituent effect
RSC Advances, (6): 61837-61847. 2016. 10.1039/c6ra14837a

Adeowo, F. Y.; Honarpourvar, B.; Skelton, A. A.
The interaction of NOTA as a bifunctional chelator with competitive alkali metal ions: a DFT study
RSC Advances, (6): 79485-79496. 2016. 10.1039/c6ra20203a

Adhikari, S.; Palepu, N. R.; Sutradhar, D.; Shepherd, S. L.; Phillips, R. M.; Kaminsky, W.; Chandra, A. K.; Kollipara, M. R.
Neutral and cationic half-sandwich arene ruthenium, Cp^{}Rh and Cp^{*}Ir oximato and oxime complexes: Synthesis, structural, DFT and biological studies*
Journal of Organometallic Chemistry, (820): 70-81. 2016. 10.1016/j.jorgancem.2016.08.004

Adhikari, S.; Sutradhar, D.; Shepherd, S. L.; Phillips, R. M.; Chandra, A. K.; Rao, K. M.
Synthesis, structural, DFT calculations and biological studies of rhodium and iridium complexes containing azine Schiff-base ligands
Polyhedron, (117): 404-414. 2016. 10.1016/j.poly.2016.06.001

Adjieufack, A. I.; Ndassa, I. M.; Mbadcam, J. K.; Rios-Gutierrez, M.; Domingo, L. R.
Understanding the reaction mechanism of the Lewis acid (MgBr₂)-catalysed 3+2 cycloaddition reaction between C-methoxycarbonyl nitrone and 2-propen-1-ol: a DFT study
Theoretical Chemistry Accounts, (136) 2016. 10.1007/s00214-016-2028-0

Afzal, S. M.; Razvi, M. A. N.; Khan, S. A.; Osman, O. I.; Bakry, A. H.; Asiri, A. M.
Physicochemical and Nonlinear Optical Properties of Novel Environmentally Benign Heterocyclic Azomethine Dyes: Experimental and Theoretical Studies
PLoS One, (11) 2016. 10.1371/journal.pone.0161613

Agou, T.; Yanagisawa, T.; Sasamori, T.; Tokitoh, N.
Synthesis and Structure of an Iron-Bromoalumanyl Complex with a Tri-Coordinated Aluminum Center
Bulletin of the Chemical Society of Japan, (89): 1184-1186. 2016. 10.1246/bcsj.20160151

Agrawal, M.; Deval, V.; Gupta, A.; Sangala, B. R.; Prabhu, S. S.
Evaluation of structure-reactivity descriptors and biological activity spectra of 4-(6-methoxy-2-naphthyl)-2-butanone using spectroscopic techniques
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (167): 142-156. 2016.
10.1016/j.saa.2016.04.053

Ahmadinejad, N.; Tahan, A.; Tari, M. T.
Chemical structure and intra-molecular effects on NMR-NQR tensors of harmine and harmaline alkaloids
Russian Journal of Physical Chemistry A, (90): 417-419. 2016. 10.1134/s0036024416020205

Ajitha, M. J.; Huang, K. W.; Kwak, J.; Kim, H. J.; Chang, S.; Jung, Y.
A potential role of a substrate as a base for the deprotonation pathway in Rh-catalysed C-H amination of heteroarenes: DFT insights
Dalton Transactions, (45): 7980-7985. 2016. 10.1039/c6dt00686h

- Akaberi, T.; Shiri, A.; Sheikhi-Mohammareh, S.
Synthesis of new derivatives of pyridazino 6,1-c pyrimido 5,4-e 1,2,4 triazine; a novel heterocyclic system
Journal of Chemical Research: 44-46. 2016. 10.3184/174751916x14497690510968
- Akilandeswari, P. E.; Gayathri, B.; Panneerselvam, M.; Jaccob, M.; Kamil, M. G. M.; Kumar, R.
Acoustical and quantum computational investigations on the stacking phenomenon of aqueous norfloxacin antibiotic
Journal of Molecular Liquids, (221): 1133-1139. 2016. 10.1016/j.molliq.2016.06.090
- Akin, S. T.; Zamudio-Bayer, V.; Duanmu, K.; Leistner, G.; Hirsch, K.; Bulow, C.; Lawicki, A.; Terasaki, A.; von Issendorff, B.; Truhlar, D. G.; Lau, J. T.; Duncan, M. A.
Size-Dependent Ligand Quenching of Ferromagnetism in Co-3(benzene)(n)(+) Clusters Studied with X-ray Magnetic Circular Dichroism Spectroscopy
Journal of Physical Chemistry Letters, (7): 4568-4575. 2016. 10.1021/acs.jpcllett.6b01839
- Akman, F.
Spectroscopic investigation, HOMO-LUMO energies, natural bond orbital (NBO) analysis and thermodynamic properties of two-armed macroinitiator containing coumarin with DFT quantum chemical calculations
Canadian Journal of Physics, (94): 583-593. 2016. 10.1139/cjp-2016-0041
- Aksakal, F.; Shvets, N.; Khairullina, V.; Dimoglo, A.
Structural and Electronic Factors Influencing the Selective Inhibition of COX-2
Mini-Reviews in Medicinal Chemistry, (16): 579-594. 2016. 10.2174/1389557515666151016124503
- Aksamentova, T. N.; Chipanina, N. N.; Grebneva, E. A.; Timofeeva, E. N.; Bolgova, Y. I.; Trofimova, O. M.
DFT study of the 1-aryl-1-fluoro-5-methylquasilsilatrane stereoisomers. NBO and QTAIM analysis
Computational and Theoretical Chemistry, (1091): 78-84. 2016. 10.1016/j.comptc.2016.07.014
- Al-Alshaikh, M. A.; Mary, Y. S.; Panicker, C. Y.; Attia, M. I.; El-Emam, A. A.; Van Alsenoy, C.
Spectroscopic investigations and molecular docking study of 3-(1H-imidazol-1(-)yl)-1-phenylpropan-1-one, a potential precursor to bioactive agents
Journal of Molecular Structure, (1109): 131-138. 2016. 10.1016/j.molstruc.2015.12.075
- Alam, M.; Alam, M. J.; Nami, S. A. A.; Lee, D. U.; Azam, M.; Ahmad, S.
Computational and anti-tumor studies of 7a-Aza-B-homostigmast-5-eno 7a, 7-d tetrazole-3 beta-yl chloride
Journal of Molecular Structure, (1108): 411-426. 2016. 10.1016/j.molstruc.2015.12.030
- Alam, M.; Lee, D. U.
Synthesis, spectroscopic and computational studies of 2-(thiophen-2-yl)-2,3-dihydro-1H-perimidine: An enzymes inhibition study
Computational Biology and Chemistry, (64): 185-201. 2016. 10.1016/j.compbiochem.2016.06.006
- Al-Ansari, I. A. Z.
Physicochemical Properties of Derivatives of N, N-Dimethylamino-cyclic-chalcones: Experimental and Theoretical Study
Chemistryselect, (1): 2935-2944. 2016. 10.1002/slct.201600458
- Alcaide, B.; Almendros, P.; Aragoncillo, C.; Gomez-Campillos, G.; Quiros, M. T.; Soriano, E.
Tunable Metal-Catalyzed Heterocyclization Reactions of Allenic Amino Alcohols: An Experimental and Theoretical Study
Journal of Organic Chemistry, (81): 7362-7372. 2016. 10.1021/acs.joc.6b00934
- Alcalde, R.; Atilhan, M.; Trenzado, J. L.; Aparicio, S.
Physicochemical Insights on Alkylcarbonate-Alkanol Solutions
Journal of Physical Chemistry B, (120): 5015-5028. 2016. 10.1021/acs.jpcb.6b02961
- Alcazar, J. J.; Marquez, E.; Mora, J. R.; Cordova-Sintjago, T.; Chuchani, G.
Theoretical study on the mechanism of the gas-phase elimination kinetics of alkyl chloroformates
Molecular Physics, (114): 719-729. 2016. 10.1080/00268976.2015.1114163

- Alekseev, N. V.
A quantum chemical study of aluminum-nitrogen bonds in three-coordinate aluminum compounds
Journal of Structural Chemistry, (56): 1043-1050. 2016. 10.1134/s0022476615060037
- Ali, M. M.; George, G.; Ramalingam, S.; Periandy, S.; Gokulakrishnan, V.
Spectroscopic investigation and chemical properties analysis on anticancer compound; alpha,alpha,alpha,alpha-Tetrabromo-p-Xylene with computational analysis
Journal of Molecular Structure, (1106): 37-52. 2016. 10.1016/j.molstruc.2015.10.078
- Ali, S. M.; Pahan, S.; Bhattacharyya, A.; Mohapatra, P. K.
Complexation thermodynamics of diglycolamide with f-elements: solvent extraction and density functional theory analysis
Physical Chemistry Chemical Physics, (18): 9816-9828. 2016. 10.1039/c6cp00825a
- Alkorta, I.; Del Bene, J. E.; Elguero, J.
H₂XP:OH₂ Complexes: Hydrogen vs. Pnicogen Bonds
Crystals, (6) 2016. 10.3390/cryst6020019
- Alkorta, I.; Elguero, J.; Del Bene, J. E.
Boron as an Electron-Pair Donor for B center dot center dot center dot Cl Halogen Bonds
Chemphyschem, (17): 3112-3119. 2016. 10.1002/cphc.201600435
- Alkorta, I.; Elguero, J.; Del Bene, J. E.
Unusual acid-base properties of the P-4 molecule in hydrogen-, halogen-, and pnicogen-bonded complexes
Physical Chemistry Chemical Physics, (18): 32593-32601. 2016. 10.1039/c6cp06474d
- Alkorta, I.; Mata, I.; Molins, E.; Espinosa, E.
Charged versus Neutral Hydrogen-Bonded Complexes: Is There a Difference in the Nature of the Hydrogen Bonds?
Chemistry-a European Journal, (22): 9226-9234. 2016. 10.1002/chem.201600788
- Almansour, A. I.; Arumugam, N.; Kumar, R. S.; Soliman, S. M.; Altaf, M.; Ghabbour, H. A.
Synthesis, Spectroscopic, X-ray Diffraction and DFT Studies of Novel Benzimidazole Fused-1,4-Oxazepines Molecules, (21) 2016. 10.3390/molecules21060724
- Almutairi, M. S.; Manimaran, D.; Joe, I. H.; Saleh, O. A.; Attia, M. I.
Structural Properties and Biological Prediction of ((1E)-3-(1H-Imidazol-1-yl)-1-phenylpropylidene amino}oxy)(4-methylphenyl)methanone: An In Silico Approach
Symmetry-Basel, (8) 2016. 10.3390/sym8010001
- Al-Soliemy, A. M.; Osman, O. I.; Hussein, M. A.; Asiri, A. M.; El-Daly, S. A.
Fluorescence, Photophysical Behaviour and DFT Investigation of E,E-2,5-bis 2-(3-pyridyl)ethenyl pyrazine (BPEP)
Journal of Fluorescence, (26): 1199-1209. 2016. 10.1007/s10895-016-1802-7
- Al-Tamimi, A. M. S.
Electronic structure, hydrogen bonding and spectroscopic profile of a new 1,2,4-triazole-5(4H)-thione derivative: A combined experimental and theoretical (DFT) analysis
Journal of Molecular Structure, (1120): 215-227. 2016. 10.1016/j.molstruc.2016.05.029
- Alturk, S.; Avci, D.; Tamer, O.; Atalay, Y.; Sahin, O.
A cobalt (II) complex with 6-methylpicolinate: Synthesis, characterization, second- and third-order nonlinear optical properties, and DFT calculations
Journal of Physics and Chemistry of Solids, (98): 71-80. 2016. 10.1016/j.jpcs.2016.06.008
- Alvarez-Barcia, S.; Flores, J. R.
Can alumina particles be formed from Al hydroxide in the circumstellar media? A first-principles chemical study
Physical Chemistry Chemical Physics, (18): 6103-6112. 2016. 10.1039/c5cp06676j

- Al-Wabli, R. I.; Manimaran, D.; John, L.; Joe, I. H.; Haress, N. G.; Attia, M. I.
Spectroscopic Investigations, DFT Calculations, and Molecular Docking Studies of the Anticonvulsant (2E)-2- 3-(1H-Imidazol-1-yl)-1-phenylpropylidene -N-(4-methylphenyl)hydr azinecarboxamide
Journal of Spectroscopy, 2016. 10.1155/2016/8520757
- Al-Wabli, R. I.; Resmi, K. S.; Mary, Y. S.; Panicker, C. Y.; Attia, M. I.; El-Emam, A. A.; Van Alsenoy, C.
Vibrational spectroscopic studies, Fukui functions, HOMO-LUMO, NLO, NBO analysis and molecular docking study of (E)-1-(1,3-benzodioxol-5-yl)-4,4-dimethylpent-1-en-3-one, a potential precursor to bioactive agents
Journal of Molecular Structure, (1123): 375-383. 2016. 10.1016/j.molstruc.2016.07.044
- Al-Zahrani, F. A.; Arshad, M. N.; Asiri, A. M.; Mahmood, T.; Gilani, M. A.; El-Shishtawy, R. M.
Synthesis and structural properties of 2-((10-alkyl-10H-phenothiazin-3-yl)methylene) malononitrile derivatives; a combined experimental and theoretical insight
Chemistry Central Journal, (10) 2016. 10.1186/s13065-016-0158-z
- Amaiz, L. V.; Cartaya, L.; Marquez, E.; Alcazar, J. J.; Maldonado, A.; Mora, J. R.; Cordova, T.; Chuchani, G.
Thermal Decomposition Kinetics of Dicyclopentadiene-1,8-dione: The Reaction Path through Quantum Chemical Calculation
International Journal of Chemical Kinetics, (48): 812-821. 2016. 10.1002/kin.21036
- Amiraslanzadeh, S.
The Effect of Doping Different Heteroatoms on the Interaction and Adsorption Abilities of Fullerene Heteroatom Chemistry, (27): 23-31. 2016. 10.1002/hc.21284
- Amiri, S. S.; Koohi, M.; Mirza, B.
Characterizations of B and N heteroatoms as substitutional doping on structure, stability, and aromaticity of novel heterofullerenes evolved from the smallest fullerene cage C-20: a density functional theory perspective
Journal of Physical Organic Chemistry, (29): 514-522. 2016. 10.1002/poc.3573
- Amiri, S. S.; Makarem, S.; Ahmar, H.; Ashenagar, S.
Theoretical studies and spectroscopic characterization of novel 4-methyl-5-((5-phenyl-1,3,4-oxadiazol-2-yl)thio)benzene-1,2-diol
Journal of Molecular Structure, (1119): 18-24. 2016. 10.1016/j.molstruc.2016.04.053
- Anacker, T.; Tew, D. P.; Friedrich, J.
First UHF Implementation of the Incremental Scheme for Open-Shell Systems
Journal of Chemical Theory and Computation, (12): 65-78. 2016. 10.1021/acs.jctc.5b00933
- Anafcheh, M.; Khodadadi, Z.; Ektefa, F.; Ghafouri, R.
Functionalization of pentagon-pentagon edges of fullerenes by cyclic polysulfides: A DFT study
Journal of Physics and Chemistry of Solids, (92): 26-31. 2016. 10.1016/j.jpcs.2015.12.004
- Anand, M.; Fernandez, I.; Schaefer, H. F.; Wu, J. I. C.
Hydrogen Bond-Aromaticity Cooperativity in Self-Assembling 4-Pyridone Chains
Journal of Computational Chemistry, (37): 59-63. 2016. 10.1002/jcc.23976
- Anand, S.; Thekkat, K.; Waghmare, U. V.
Two-Dimensional Rectangular and Honeycomb Lattices of NbN: Emergence of Piezoelectric and Photocatalytic Properties at Nanoscale
Nano Letters, (16): 126-131. 2016. 10.1021/acs.nanolett.5b03275
- Ananyev, I. V.; Lyssenko, K. A.
A chemist's point of view: the noncylindrical symmetry of electron density means nothing but still means something
Mendeleev Communications, (26): 338-340. 2016. 10.1016/j.mencom.2016.07.024
- Andrade, D. M.; Holzmann, N.; Frenking, G.
Bonding analysis of ylidone complexes EL2 ($E = C-Pb$) with phosphine and carbene ligands L
Canadian Journal of Chemistry, (94): 1006-1014. 2016. 10.1139/cjc-2016-0263

- Andrez, J.; Pecaut, J.; Scopelliti, R.; Kefalidis, C. E.; Maron, L.; Rosenzweig, M. W.; Meyere, K.; Mazzanti, M.
Synthesis and reactivity of a terminal uranium(IV) sulfide supported by siloxide ligands
Chemical Science, (7): 5846-5856. 2016. 10.1039/c6sc00675b
- Anez, R.; Sierraalta, A.; Coll, D.; Castellanos, O.; Soscun, H.
Moller-Plesset 2 and density functional theory studies of the interaction between aromatic compounds and Zn-porphyrins
Computational and Theoretical Chemistry, (1084): 133-139. 2016. 10.1016/j.comptc.2016.03.024
- Aniola, M.; Dega-Szafran, Z.; Katrusiak, A.; Komasa, A.; Szafran, M.
Disproportional proton tautomers of pipelicolic acid and 2,6-dichloro-4-nitrophenol in a 2:3 complex
Chemical Physics, (477): 88-95. 2016. 10.1016/j.chemphys.2016.08.030
- Aniola, M.; Dega-Szafran, Z.; Katrusiak, A.; Komasa, A.; Szafran, M.
Synthesis, spectroscopic and theoretical studies of (R/S)-piperidinium-3-carboxylic acid 2,6-dichloro-4-nitrophenolate
Vibrational Spectroscopy, (83): 46-56. 2016. 10.1016/j.vibspec.2016.01.003
- Ansari, S. A.; Mohapatra, P. K.; Ali, S. M.; Sengupta, A.; Bhattacharyya, A.; Verboom, W.
Understanding the complexation of Eu³⁺ with three diglycolamide-functionalized calix 4 arenes: spectroscopic and DFT studies
Dalton Transactions, (45): 5425-5429. 2016. 10.1039/c6dt00180g
- Aono, S.; Mori, T.; Sakaki, S.
3D-RISM-MP2 Approach to Hydration Structure of Pt(II) and Pd(II) Complexes: Unusual H-Ahead Mode vs Usual O-Ahead One
Journal of Chemical Theory and Computation, (12): 1189-1206. 2016. 10.1021/acs.jctc.5b01137
- Applewhite, M. J.; Haynes, D. A.; Arnott, G. E.
Cyanocalix 4 arenes: synthesis, crystal structures and reactivity studies
Supramolecular Chemistry, (28): 475-484. 2016. 10.1080/10610278.2015.1121268
- Arabieh, M.; Platas-Iglesias, C.
A density functional theory study on the interaction of dipicolinic acid with hydrated Fe²⁺ cation
Computational and Theoretical Chemistry, (1090): 134-146. 2016. 10.1016/j.comptc.2016.06.010
- Arakawa, M.; Yamane, R.; Terasaki, A.
Reaction Sites of CO on Size-Selected Silicon Oxide Cluster Anions: A Model Study of Chemistry in the Interstellar Environment
Journal of Physical Chemistry A, (120): 139-144. 2016. 10.1021/acs.jpca.5b08900
- Aravena, D.; Atanasov, M.; Neese, F.
Periodic Trends in Lanthanide Compounds through the Eyes of Multireference ab Initio Theory
Inorganic Chemistry, (55): 4457-4469. 2016. 10.1021/acs.inorgchem.6b00244
- Archirel, P.; Berge, J.; Houee-Levin, C.
Radical Cations of the Monomer and van der Waals Dimer of a Methionine Residue as Prototypes of (2 Center-3 Electron) SN and SS Bonds. Molecular Simulations of Their Absorption Spectra in Water
Journal of Physical Chemistry B, (120): 9875-9886. 2016. 10.1021/acs.jpcb.6b06329
- Ardizzoia, G. A.; Bea, M.; Brenna, S.; Therrien, B.
A Quantitative Description of the sigma-Donor and pi-Acceptor Properties of Substituted Phenanthrolines
European Journal of Inorganic Chemistry: 3829-3837. 2016. 10.1002/ejic.201600647
- Ari, H.; Ozpozan, T.
Nonionic and zwitterionic forms of glycylglycylarginine as a part of spider silk protein: Spectroscopic and theoretical study

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (152): 557-571. 2016.
10.1016/j.saa.2014.12.115

Ari, H.; Ozpozan, T.; Buyukmumcu, Z.; Kabacali, Y.; Sacmaci, M.
Theoretical and vibrational spectroscopic approach to keto-enol tautomerism in methyl-1-(4-methoxybenzoyl)-3-(4-methoxyphenyl)-3-oxopropanoylcarbamate
Journal of Molecular Structure, (1122): 48-61. 2016. 10.1016/j.molstruc.2016.05.060

Ariafard, A.; Ghari, H.; Khaledi, Y.; Bagi, A. H.; Wierenga, T. S.; Gardiner, M. G.; Canty, A. J.
Theoretical Investigation into the Mechanism of Cyanomethylation of Aldehydes Catalyzed by a Nickel Pincer Complex in the Absence of Base Additives
ACS Catalysis, (6): 60-68. 2016. 10.1021/acscatal.5b01642

Arjunan, V.; Anitha, R.; Thenmozhi, S.; Marchewka, M. K.; Mohan, S.
Potential energy profile, structural, vibrational and reactivity descriptors of trans-2-methoxycinnamic acid by FTIR, FT-Raman and quantum chemical studies
Journal of Molecular Structure, (1113): 42-54. 2016. 10.1016/j.molstruc.2016.02.034

Arkan, F.; Izadyar, M.
Quantum chemical aspects of solvent effects on the Diels-Alder reaction of 2,3-dimethyl-1,3-butadiene and diethyl azodicarboxylate
Progress in Reaction Kinetics and Mechanism, (41): 224-234. 2016. 10.3184/146867816x14702227410256

Arkan, F.; Izadyar, M.; Nakhaeipour, A.
The role of the electronic structure and solvent in the dye-sensitized solar cells based on Zn-porphyrins: Theoretical study
Energy, (114): 559-567. 2016. 10.1016/j.energy.2016.08.027

Arlt, S.; Harloff, J.; Schulz, A.; Stoffers, A.; Villinger, A.
Cyanido Antimonate(III) and Bismuthate(III) Anions
Inorganic Chemistry, (55): 12321-12328. 2016. 10.1021/acs.inorgchem.6b02174

Armengol, P.; Gelabert, R.; Moreno, M.; Lluch, J. M.
Chromophore interactions leading to different absorption spectra in mNeptune1 and mCardinal red fluorescent proteins
Physical Chemistry Chemical Physics, (18): 16964-16976. 2016. 10.1039/c6cp01297c

Aronoff, M. R.; Gold, B.; Raines, R. T.
Rapid cycloaddition of a diazo group with an unstrained dipolarophile
Tetrahedron Letters, (57): 2347-2350. 2016. 10.1016/j.tetlet.2016.04.020

Arora, R.; Kakkar, R.
Theoretical study of the mechanism of the Wolff rearrangement of some diazocarbonyl compounds
Computational and Theoretical Chemistry, (1094): 32-41. 2016. 10.1016/j.comptc.2016.08.020

Arpa, E. M.; Frias, M.; Alvarado, C.; Aleman, J.; Diaz-Tendero, S.
Weakly bounded intermediates as a previous step toward's highly-enantioselective iminium type additions of beta-keto-sulfoxides and -sulfones
Journal of Molecular Catalysis a-Chemical, (423): 308-318. 2016. 10.1016/j.molcata.2016.03.013

Arras, J.; Eichele, K.; Maryasin, B.; Schubert, H.; Ochsenfeld, C.; Wesemann, L.
Intermolecular Sn-119,P-31 Through-Space Spin-Spin Coupling in a Solid Bivalent Tin Phosphido Complex
Inorganic Chemistry, (55): 4669-4675. 2016. 10.1021/acs.inorgchem.6b00573

Arshad, J.; Hoffmann, A.; Gesing, S.; Grunzke, R.; Kruger, J.; Kiss, T.; Herres-Pawlits, S.; Terstyanszky, G.
Multi-level meta-workflows: new concept for regularly occurring tasks in quantum chemistry
Journal of Cheminformatics, (8) 2016. 10.1186/s13321-016-0169-8

- Arshadi, S.; Pourkhiz, F.
NBO, AIM, and TD-DFT assisted screening of BNNT optimum diameter on ethyl phosphorodimethylamidocyanide sensor design
Phosphorus Sulfur and Silicon and the Related Elements, (191): 1013-1021. 2016. 10.1080/10426507.2015.1130045
- Arz, M. I.; Schnakenburg, G.; Meyer, A.; Schiemann, O.; Filippou, A. C.
The Si₂H radical supported by two N-heterocyclic carbenes
Chemical Science, (7): 4973-4979. 2016. 10.1039/c6sc01569g
- Arz, M. I.; Strassmann, M.; Geiss, D.; Schnakenburg, G.; Filippou, A. C.
Addition of Small Electrophiles to N-Heterocyclic-Carbene-Stabilized Disilicon(0): A Revisit of the Isolobal Concept in Low-Valent Silicon Chemistry
Journal of the American Chemical Society, (138): 4589-4600. 2016. 10.1021/jacs.6b01018
- Asath, R. M.; Rekha, T. N.; Premkumar, S.; Mathavan, T.; Benial, A. M. F.
Vibrational, spectroscopic, molecular docking and density functional theory studies on N-(5-aminopyridin-2-yl)acetamide
Journal of Molecular Structure, (1125): 633-642. 2016. 10.1016/j.molstruc.2016.07.064
- Asath, R. M.; Rekha, T. N.; Rajkumar, B. J. M.; Premkumar, S.; Jawahar, A.; Mathavan, T.; Benial, A. M. F.
Conformational, vibrational spectroscopic, nonlinear optical activity, and structure-activity studies on 2-hydroxy-3,5-dinitropyridine: Combined experimental and density functional theory approach
Spectroscopy Letters, (49): 155-166. 2016. 10.1080/00387010.2015.1111242
- Asatryan, R.; Ruckenstein, E.
Effect of "Reducible" Titania Promotion on the Mechanism of H-Migration in Pd/SiO₂ Clusters
Catalysis Letters, (146): 398-423. 2016. 10.1007/s10562-015-1642-0
- Asiri, A. M.; Ersanli, C. C.; Sahin, O.; Arshad, M. N.; Hameed, S. A.
Molecular structure, spectroscopic and quantum chemical studies of 1',3',3'-trimethylspiro benzo f chromene-3,2'-indoline
Journal of Molecular Structure, (1111): 108-117. 2016. 10.1016/j.molstruc.2016.01.086
- Astani, E.; Heshmati, E.; Chen, C. J.; Hadipour, N. L.; Shekarsaraei, S.
A study of hydrogen bond effects on the oxygen, nitrogen, and hydrogen electric field gradient tensors in the active site of human dehydroepiandrosterone sulphotransferase: A density-functional theory based treatment
Chemical Physics Letters, (653): 78-84. 2016. 10.1016/j.cplett.2016.04.001
- Astani, E. K.; Heshmati, E.; Chen, C. J.; Hadipour, N. L.
A theoretical study on the characteristics of the intermolecular interactions in the active site of human androsterone sulphotransferase: DFT calculations of NQR and NMR parameters and QTAIM analysis
Journal of Molecular Graphics & Modelling, (68): 14-22. 2016. 10.1016/j.jmgm.2016.06.002
- Asthagiri, D.; Ballal, D.; Venkataraman, P.; Fouad, W. A.; Cox, K. R.; Chapman, W. G.
Response to "Comment on 'Isolating the non-polar contributions to the intermolecular potential for water-alkane interactions'" J. Chem. Phys. 144, 137101 (2016)
Journal of Chemical Physics, (144) 2016. 10.1063/1.4944979
- Atabaki, H.; Nori-Shargh, D.; Momen-Heravi, M.; Niazi, A.
Electrostatic and stereoelectronic interaction impacts on the structural properties and isomerization reactions of methyl isocyanide and its trihalo-analogs
Structural Chemistry, (27): 883-896. 2016. 10.1007/s11224-015-0653-1
- Attar, S.; Espa, D.; Artizzu, F.; Mercuri, M. L.; Serpe, A.; Sessini, E.; Concas, G.; Congiu, F.; Marchio, L.; Deplano, P.
A Platinum-Dithiolene Monoanionic Salt Exhibiting Multiproperties, Including Room-Temperature Proton-Dependent Solution Luminescence
Inorganic Chemistry, (55): 5118-5126. 2016. 10.1021/acs.inorgchem.5b02491

- Attia, A. A. A.; Lulan, A.; King, R. B.
Novel non-spherical deltahedra in trirhenaborane structures
New Journal of Chemistry, (40): 7564-7572. 2016. 10.1039/c6nj01922f
- Aurell, M. J.; Domingo, L. R.; Arno, M.; Zaragoza, R. J.
A DFT study of the mechanism of NHC catalysed annulation reactions involving alpha,beta-unsaturated acyl azoliums and beta-naphthol
Organic & Biomolecular Chemistry, (14): 8338-8345. 2016. 10.1039/c6ob01442a
- Autschbach, J.
Orbitals for Analyzing Bonding and Magnetism of Heavy-Metal Complexes
Comments on Inorganic Chemistry, (36): 215-244. 2016. 10.1080/02603594.2015.1121874
- Avendano, M.; Cordova, T.; Mora, J. R.; Chuchani, G.
Quantum chemical theory calculations on the mechanism of the homogeneous, unimolecular gas-phase elimination kinetics of selected diazirines
Computational and Theoretical Chemistry, (1078): 23-29. 2016. 10.1016/j.comptc.2015.12.008
- Ayoub, M.
Energy landscape of nonconventional hydrogen bonding: Natural bond orbital study
Abstracts of Papers of the American Chemical Society, (252) 2016.
- Ayoub, N. A.; Browne, A. R.; Anderson, B. L.; Gray, T. G.
Cyclometalated gold(III) trioxadiborrin complexes: studies of the bonding and excited states
Dalton Transactions, (45): 3820-3830. 2016. 10.1039/c5dt04732c
- Azam, M.; Velmurugan, G.; Wabaidur, S. M.; Trzesowska-Kruszynska, A.; Kruszynski, R.; Al-Resayes, S. I.; Al-Othman, Z. A.; Venuvanalingam, P.
Structural elucidation and physicochemical properties of mononuclear Uranyl(VI) complexes incorporating dianionic units
Scientific Reports, (6) 2016. 10.1038/srep32898
- Baggioli, A.; Cavallotti, C. A.; Famulari, A.
Exploring short intramolecular interactions in alkylaromatic substrates
Physical Chemistry Chemical Physics, (18): 29616-29628. 2016. 10.1039/c6cp03323g
- Bagheri, S.; Masoodi, H. R.; Yousofvand, A.
Exploring the role of substituents on cooperativity between N center dot center dot center dot HF and CH center dot center dot center dot F hydrogen bonds in ternary systems involving aromatic azine: Substituted complexes of s-triazine:HF:s-triazine as a working model
Computational and Theoretical Chemistry, (1092): 12-18. 2016. 10.1016/j.comptc.2016.07.002
- Bahrami, H.; Farhadi, S.; Siadatnasab, F.
Non-bonding interactions and non-covalent delocalization effects play a critical role in the relative stability of group 12 complexes arising from interaction of diethanolthiocarbamate with the cations of transition metals Zn(II), Cd(II), and Hg(II): a theoretical study
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3008-y
- Bahrami, H.; Jaferian, G.; Davari, M. D.; Zahedi, M.; Moosavi-Movahedi, A. A.
The Theoretical and Experimental Studies on Oxidation of Straight Chain Amino Acids in Moderately Concentrated Sulfuric Acid Medium
International Journal of Chemical Kinetics, (48): 647-659. 2016. 10.1002/kin.21014
- Bahring, S.; Martin-Gomis, L.; Olsen, G.; Nielsen, K. A.; Kim, D. S.; Duedal, T.; Sastre-Santos, A.; Jeppesen, J. O.; Sessler, J. L.
Design and Sensing Properties of a Self-Assembled Supramolecular Oligomer
Chemistry-a European Journal, (22): 1958-1967. 2016. 10.1002/chem.201503701
- Bai, S. M.; Barbatti, M.

Why Replacing Different Oxygens of Thymine with Sulfur Causes Distinct Absorption and Intersystem Crossing
Journal of Physical Chemistry A, (120): 6342-6350. 2016. 10.1021/acs.jpca.6b05110

Baker, M. B.; Ferreira, R. B.; Tasserou, J.; Lampkins, A. J.; Al Abbas, A.; Abboud, K. A.; Castellano, R. K.
Selective and Sequential Aminolysis of Benzotrifuranone: Synergism of Electronic Effects and Ring Strain Gradient
Journal of Organic Chemistry, (81): 9279-9288. 2016. 10.1021/acs.joc.6b01867

Bakirdere, E. G.; Fellah, M. F.; Canpolat, E.; Kaya, M.; Gur, S.
Design, synthesis, characterization, and antimicrobial activity of the new 2-{(E)- (4-aminophenyl)imino methyl}-4,6-dichlorophenol and its complexes with Co(II), Ni(II), Cu(II) and Zn(II): An experimental and DFT study
Journal of the Serbian Chemical Society, (81): 509-520. 2016. 10.2298/jsc151030008b

Bakkiyaraj, D.; Periandy, S.; Xavier, S.
Molecular structural investigation of adenosine using spectroscopic and quantum computational calculations
Journal of Molecular Structure, (1119): 490-504. 2016. 10.1016/j.molstruc.2016.04.096

Bakkiyaraj, D.; Periandy, S.; Xavier, S.
Spectroscopic (FT-IR, FT-Raman, FT-NMR and UV-Vis) investigation on benzil dioxime using quantum computational methods
Journal of Molecular Structure, (1108): 33-45. 2016. 10.1016/j.molstruc.2015.11.044

Bako, I.; Mayer, I.
On Dipole Moments and Hydrogen Bond Identification in Water Clusters
Journal of Physical Chemistry A, (120): 4408-4417. 2016. 10.1021/acs.jpca.6b03187

Bakr, B. W.; Sherrill, C. D.
Analysis of transition state stabilization by non-covalent interactions in the Houk-List model of organocatalyzed intermolecular Aldol additions using functional-group symmetry-adapted perturbation theory
Physical Chemistry Chemical Physics, (18): 10297-10308. 2016. 10.1039/c5cp07281f

Bakthavachalam, K.; Yuvaraj, K.; Zafar, M.; Ghosh, S.
Reactivity of M-2(mu-Cl)(2)(cod)(2) (M=Ir, Rh) and Ru(Cl)(2)(cod)(CH3CN)(2) with Na H2B(bt)(2) : Formation of Agostic versus Borate Complexes
Chemistry-a European Journal, (22): 17291-17297. 2016. 10.1002/chem.201603480

Balachandar, S.; Sethuram, M.; Muthuraja, P.; Shanmugavadi, T.; Dhandapani, M.
Ligand based pharmacophoric modelling and docking of bioactive pyrazolium 3-nitrophthalate (P3NP) on Bacillus subtilis, Aspergillus fumigatus and Aspergillus niger - Computational and Hirshfeld surface analysis
Journal of Photochemistry and Photobiology B-Biology, (163): 352-365. 2016. 10.1016/j.jphotobiol.2016.08.045

Balachander, R.; Manimekalai, A.
Synthesis, conformational and theoretical studies of 1,n-di(2-formyl-4-phenylazophenoxy)alkanes
Journal of Molecular Structure, (1104): 70-78. 2016. 10.1016/j.molstruc.2015.10.006

Balamurugan, N.; Sampathkrishnan, S.; Charanya, C.
Natural Bond Orbitals (NBO), Natural Population Analysis, Mulliken Analysis of Atomic Charges of 2- (2, 3-Dimethylphenyl) Amino Benzoic Acid
Spectroscopy and Spectral Analysis, (36): 1273-1276. 2016. 10.3964/j.issn.1000-0593(2016)04-1273-04

Balcells, D.
Insight into Metal-Catalyzed Water Oxidation from a DFT Perspective
Advances in Organometallic Chemistry, Vol 65, (65): 115-173. 2016. 10.1016/bs.adomc.2016.01.001

Balcells, D.; Eisenstein, O.; Tilset, M.; Nova, A.
Coordination and insertion of alkenes and alkynes in Au-III complexes: nature of the intermediates from a computational perspective
Dalton Transactions, (45): 5504-5513. 2016. 10.1039/c5dt05014f

Balci, K.; Akkaya, Y.; Akyuz, S.; Collier, W. B.; Stricker, M. C.; Stover, D. D.; Ritzhaupt, G.; Koch, A.; Kleinpeter, E.
The effects of conformation and zwitterionic tautomerism on the structural and vibrational spectral data of anserine
Vibrational Spectroscopy, (86): 277-289. 2016. 10.1016/j.vibspec.2016.08.003

Balci, V.; Uzun, A.
Understanding Spectroscopic Features of Trihexyltetradecylphosphonium Chloride
Chemistryselect, (1): 741-747. 2016. 10.1002/slct.201600067

Banerjee, P.; Bhattacharya, I.; Chakraborty, T.
Matrix isolation infrared spectra of O-H center dot center dot center pi Hydrogen bonded complexes of Acetic acid and Trifluoroacetic acid with Benzene
Journal of Chemical Sciences, (128): 1549-1555. 2016. 10.1007/s12039-016-1165-2

Banerjee, P.; Bhattacharya, I.; Chakraborty, T.
Matrix Isolation Infrared Spectroscopy of an O-H center dot center dot center pi Hydrogen-Bonded Complex between Formic Acid and Benzene
Journal of Physical Chemistry A, (120): 3731-3739. 2016. 10.1021/acs.jpca.6b03447

Bani-Yaseen, A. D.
Computational insights into the photocyclization of diclofenac in solution: effects of halogen and hydrogen bonding
Physical Chemistry Chemical Physics, (18): 21322-21330. 2016. 10.1039/c6cp03671f

Banu, T.; Ghosh, A.; Das, A. K.
Impact of metal-alkoxide functionalized linkers on H-2 binding: A density functional study
Chemical Physics Letters, (658): 140-145. 2016. 10.1016/j.cplett.2016.06.037

Barabas, J.; Holtzl, T.
Reaction of N2O and CO Catalyzed with Small Copper Clusters: Mechanism and Design
Journal of Physical Chemistry A, (120): 8862-8870. 2016. 10.1021/acs.jpca.6b08349

Bardakci, T.; Kumru, M.; Altun, A.
Molecular structures, charge distributions, and vibrational analyses of the tetracoordinate Cu(II), Zn(II), Cd(II), and Hg(II) bromide complexes of p-toluidine investigated by density functional theory in comparison with experiments
Journal of Molecular Structure, (1116): 292-302. 2016. 10.1016/j.molstruc.2016.03.023

Baryshnikova, S. V.; Bellan, E. V.; Poddel'sky, A. I.; Fukin, G. K.; Abakumov, G. A.
The synthesis and structure of new tin(II) complexes based on ferrocenyl-containing o-iminophenols
Inorganic Chemistry Communications, (69): 94-97. 2016. 10.1016/j.inoche.2016.05.003

Basheer, S. M.; Sreekanth, A.
TD-DFT study on the fluoride and copper ion sensing mechanism of pyrene N(4) phenyl thiosemicarbazone
Computational and Theoretical Chemistry, (1085): 31-39. 2016. 10.1016/j.comptc.2016.03.035

Basheer, S. M.; Willis, A. C.; Pace, R. J.; Sreekanth, A.
Spectroscopic and TD-DFT studies on the turn-off fluorescent chemosensor based on anthraldehyde N(4) cyclohexyl thiosemicarbazone for the selective recognition of fluoride and copper ions
Polyhedron, (109): 7-18. 2016. 10.1016/j.poly.2016.01.021

Baskar, A. J. A.; Rajpurohit, A. S.; Panneerselvam, M.; Singh, D. R.; Kannappan, V.; Jaccob, M.
Application of ultrasound in assessing strength of molecular non-covalent interactions in ternary liquid mixtures
Journal of Molecular Liquids, (222): 703-710. 2016. 10.1016/j.molliq.2016.07.105

Batebi, H.; Imhof, P.
Phosphodiester hydrolysis computed for cluster models of enzymatic active sites
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-2020-8

Bauza, A.; Frontera, A.

On the Versatility of BH₂X (X=F, Cl, Br, and I) Compounds as Halogen-, Hydrogen-, and Triel-Bond Donors: An AbInitio Study
Chemphyschem, (17): 3181-3186. 2016. 10.1002/cphc.201600683

Bauza, A.; Frontera, A.
RCH₃ center dot center dot center O Interactions in Biological Systems: Are They Trifurcated H-Bonds or Noncovalent Carbon Bonds?
Crystals, (6) 2016. 10.3390/cryst6030026

Bauza, A.; Mooibroek, T. J.; Frontera, A.
sigma-Hole Opposite to a Lone Pair: Unconventional Pnicogen Bonding Interactions between ZF(3) (Z=N, P, As, and Sb) Compounds and Several Donors
Chemphyschem, (17): 1608-1614. 2016. 10.1002/cphc.201600073

Bauza, A.; Mooibroek, T. J.; Frontera, A.
Tetrel Bonding Interactions
Chemical Record, (16): 473-487. 2016. 10.1002/tcr.201500256

Bayach, I.; Achari, V. M.; Iskandar, W.; Sugimura, A.; Hashim, R.
Computational insights into octyl-D-xyloside isomers towards understanding the liquid crystalline structure: physico-chemical features
Liquid Crystals, (43): 1503-1513. 2016. 10.1080/02678292.2016.1185173

Bayat, M.; Ahmadian, N.
Theoretical studies on structures, stability and nature of C->E (E = Si, Sn) bond in some derivatives of bitriazole-base NHC complexes with five-membered chelate rings
Journal of the Iranian Chemical Society, (13): 397-402. 2016. 10.1007/s13738-015-0748-z

Bayat, M.; Amraie, F.; Salehzadeh, S.
Theoretical studies on structure, formation and nature of bond in a Disila-, Digerma- and distannacyclobutene ring
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500322

Bayat, M.; Ebrahimkhani, L.; Salehzadeh, S.
Where, how and how much the strength of interaction between a hydrated lanthanide cation and a pi-system would be increased? A theoretical study
Journal of Molecular Liquids, (218): 59-67. 2016. 10.1016/j.molliq.2016.02.008

Bayat, M.; Hatami, M.
Nature of the metal-ligand bond in some (CO)(4)M <- BIIM(R) {M = Cr, Mo, W; R = H, F, Cl, Br} complexes: A theoretical study
Polyhedron, (110): 46-54. 2016. 10.1016/j.poly.2016.02.022

Bayat, M.; Kamali, S.
Computational landscape of the formation and nature of bond in the "1+1" versus "1+2" nano-sized complexes of some adducts of N-heterocyclic carbenes (NHC) with heavy elements of group II (Ca, Sr, Ba) metallocenes
Journal of Molecular Liquids, (222): 953-962. 2016. 10.1016/j.molliq.2016.07.097

Beaula, T. J.; Muthuraja, P.; Dhandapani, M.; Joe, I. H.; Rastogi, V. K.; Jothy, V. B.
Biological applications and spectroscopic investigations of 4-nitrophenol-urea dimer: A DFT approach
Chemical Physics Letters, (645): 59-70. 2016. 10.1016/j.cplett.2015.12.029

Bechaieb, R.; Ben Akacha, A.; Gerard, H.
Quantum chemistry insight into Mg-substitution in chlorophyll by toxic heavy metals: Cd, Hg and Pb
Chemical Physics Letters, (663): 27-32. 2016. 10.1016/j.cplett.2016.09.053

Bednarko, J.; Wielinska, J.; Sikora, K.; Liberek, B.; Nowacki, A.
Theoretical studies on the reaction of mono- and ditriflate derivatives of 1,4:3,6-dianhydro-D-mannitol with trimethylamine-Can a quaternary ammonium salt be a source of the methyl group?

Journal of Computer-Aided Molecular Design, (30): 13-26. 2016. 10.1007/s10822-015-9885-9

Begum, S.; Subramanian, R.

A theoretical investigation of the energetics and spectroscopic properties of the gas-phase linear proton-bound cation-molecule complexes, XCH+-N-2 (X = O, S)

Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-015-2866-z

Behjatmanesh-Ardakani, R.; Pourroustaei-Ardakani, F.; Taghdiri, M.; Kotena, Z. M.

DFT-B3LYP study of interactions between host biphenyl-1-aza-18-crown-6 ether derivatives and guest Cd²⁺: NBO, NEDA, and QTAIM analyses

Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3012-2

Behzadi, H.; Khalilnia, Z.

Aromatic-like behavior of germanium nanocrystals

RSC Advances, (6): 47434-47442. 2016. 10.1039/c6ra02635d

Beiginejad, H.; Nematollahi, D.; Khazalpour, S.

Mechanistic Study of Electrochemical Oxidation of 4-Morpholinoaniline in Aqueous Solution: Experimental and Theoretical Studies

Journal of the Electrochemical Society, (163): I1234-I1239. 2016. 10.1149/2.1081603jes

Benallou, A.; El Abdallaoui, H. E.; Garmes, H.

A conceptual DFT approach towards analysing feasibility of the intramolecular cycloaddition Diels-Alder reaction of triene amide in Lewis acid catalyst

Journal of Chemical Sciences, (128): 1489-1496. 2016. 10.1007/s12039-016-1138-5

Benallou, A.; El Abdallaoui, H. E.; Garmes, H.

Effect of hydrogen bonding on the intramolecular cycloaddition Diels-Alder reaction of triene-amide in an aqueous solution (case of a single molecule of water)

Tetrahedron, (72): 76-83. 2016. 10.1016/j.tet.2015.10.078

Benhalima, N.; Boukabcha, N.; Tamer, O.; Chouaih, A.; Avci, D.; Atalay, Y.; Hamzaoui, F.

Solvent Effects on Molecular Structure, Vibrational Frequencies, and NLO Properties of N-(2,3-Dichlorophenyl)-2-Nitrobenzene-Sulfonamide: a Density Functional Theory Study

Brazilian Journal of Physics, (46): 371-383. 2016. 10.1007/s13538-016-0419-2

Bennett, S. D.; Pope, S. J. A.; Jenkins, R. L.; Ward, B. D.

Scandium Complexes Bearing Bis(oxazolinylphenyl)amide Ligands: An Analysis of Their Reactivity, Solution-State Structures and Photophysical Properties

European Journal of Inorganic Chemistry: 2932-2941. 2016. 10.1002/ejic.201600223

Bensalem, N.; Zouchoune, B.

Coordination capabilities of anthracene ligand in binuclear sandwich complexes: DFT investigation

Structural Chemistry, (27): 1781-1792. 2016. 10.1007/s11224-016-0798-6

Bentz, E. N.; Pomilio, A. B.; Lobayan, R. M.

Z-Isomers of (4 alpha -> 6 ", 2 alpha -> O -> 1 ")-phenylflavan substituted with R '=R=OH. Conformational properties, electronic structure and aqueous solvent effects

Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3034-9

Berezin, D. B.; Talanova, A. E.; Krest'yaninov, M. A.; Serov, I. N.; Semeikin, S.

Solvent-Dependent Tautomerism of the Inverted Isomer of meso-Tetraphenylporphine: Effect of the Polarity of the Medium

Russian Journal of Physical Chemistry A, (90): 1948-1955. 2016. 10.1134/s0036024416100058

Berg, L.; Mishra, B. K.; Andersson, C. D.; Ekstrom, F.; Linusson, A.

The Nature of Activated Non-classical Hydrogen Bonds: A Case Study on Acetylcholinesterase-Ligand Complexes

Chemistry-a European Journal, (22): 2672-2681. 2016. 10.1002/chem.201503973

- Bernes, S.; Melendez, F. J.; Torrens, H.
Cis-trans isomerism in a square-planar platinum(II) complex bearing bulky fluorinated phosphane ligands
Acta Crystallographica Section C-Structural Chemistry, (72): 268-. 2016. 10.1107/s2053229616003132
- Berry, E.; Gomes, G. D.; MacLean, A.; Martin, J. R.; Wiget, P. A.
Discovery of a Long-Range Perlin Effect in a Conformationally Constrained Oxocane
Journal of Organic Chemistry, (81): 5740-5744. 2016. 10.1021/acs.joc.6b00819
- Bhabak, K. P.; Bhowmick, D.
Synthetic strategies of gold(II)-selenolates from ortho-substituted diaryl diselenides via selenol and selenenyl sulfide intermediates
Inorganica Chimica Acta, (450): 337-345. 2016. 10.1016/j.ica.2016.06.022
- Bhakhoa, H.; Rhyman, L.; Lee, E. P. F.; Ramasami, P.; Dyke, J. M.
Can Cyclen Bind Alkali Metal Azides? A DFT Study as a Precursor to Synthesis
Chemistry-a European Journal, (22): 4469-4482. 2016. 10.1002/chem.201504607
- Bharatam, P. V.; Arfeen, M.; Patel, N.; Jain, P.; Bhatia, S.; Chakraborti, A. K.; Khullar, S.; Gupta, V.; Mandal, S. K.
Design, Synthesis, and Structural Analysis of Divalent NI Compounds and Identification of a New Electron-Donating Ligand
Chemistry-a European Journal, (22): 1088-1096. 2016. 10.1002/chem.201503618
- Bhattacharyya, S.; Roy, V. P.; Wategaonkar, S.
Acid-Base Formalism Extended to Excited State for O-H center dot center dot center dot S Hydrogen Bonding Interaction
Journal of Physical Chemistry A, (120): 6902-6916. 2016. 10.1021/acs.jpca.6b04396
- Bichara, L. C.; Alvarez, P. E.; Bimbi, M. V. F.; Vaca, H.; Gervasi, C.; Brandan, S. A.
Structural and spectroscopic study of a pectin isolated from citrus peel by using FTIR and FT-Raman spectra and DFT calculations
Infrared Physics & Technology, (76): 315-327. 2016. 10.1016/j.infrared.2016.03.009
- Billes, F.; Ziegler, I.; Mikosch, H.
Vibrational spectroscopic study of sodium-1,2,4-triazole, an important intermediate compound in the synthesis of several active substances
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (153): 349-362. 2016.
10.1016/j.saa.2015.08.014
- Binder, J. F.; Corrente, A. M.; Macdonald, C. L. B.
A simple route to phosphamethine cyanines from S,N-heterocyclic carbenes
Dalton Transactions, (45): 2138-2147. 2016. 10.1039/c5dt03019f
- Bistoni, G.; Belpassi, L.; Tarantelli, F.
Advances in Charge Displacement Analysis
Journal of Chemical Theory and Computation, (12): 1236-1244. 2016. 10.1021/acs.jctc.5b01166
- Bistoni, G.; Rampino, S.; Scafuri, N.; Ciancaleoni, G.; Zuccaccia, D.; Belpassi, L.; Tarantelli, F.
How pi back-donation quantitatively controls the CO stretching response in classical and non-classical metal carbonyl complexes
Chemical Science, (7): 1174-1184. 2016. 10.1039/c5sc02971f
- Biswas, S.; Roy, P.; Sarkar, D.; Mondal, T. K.
Ruthenium carbonyl complex bearing thioether containing Schiff base ligand: Structure, electrochemistry and catalytic activity
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (55): 929-937. 2016.

Blackburn, B.; Crane, J. H.; Knapp, C. E.; Powell, M. J.; Marchand, P.; Pugh, D.; Bear, J. C.; Parkin, I. P.; Carmalt, C. J.
Reactivity of vanadium oxytrichloride with beta-diketones and diesters as precursors for vanadium nitride and carbide
Materials & Design, (108): 780-790. 2016. 10.1016/j.matdes.2016.06.029

Blanco, S.; Pinacho, P.; Lopez, J. C.
Hydrogen-Bond Cooperativity in Formamide(2)-Water: A Model for Water-Mediated Interactions
Angewandte Chemie-International Edition, (55): 9331-9335. 2016. 10.1002/anie.201603319

Blass, B. L.; Sanchez, R. H.; Decker, V. A.; Robinson, M. J.; Piro, N. A.; Kassel, W. S.; Diaconescu, P. L.; Nataro, C.
Structural, Computational, and Spectroscopic Investigation of Pd(κ (3)-1,1'-bis(di-tert-butylphosphino)ferrocenediyl)X (+) (X = Cl, Br, I) Compounds
Organometallics, (35): 462-470. 2016. 10.1021/acs.organomet.5b00889

Bogdan, E.; Verneuil, A. Q.; Besseau, F.; Compain, G.; Linclau, B.; Le Questel, J. Y.; Graton, J.
 α -Fluoro-o-cresols: The Key Role of Intramolecular Hydrogen Bonding in Conformational Preference and Hydrogen-Bond Acidity
Chemphyschem, (17): 2702-2709. 2016. 10.1002/cphc.201600453

Bohme, U.; Gerwig, M.; Grundler, F.; Brendler, E.; Kroke, E.
Unexpected Formation and Crystal Structure of the Highly Symmetric Carbanion C(SiCl₃)₃ (-)
European Journal of Inorganic Chemistry: 5028-5035. 2016. 10.1002/ejic.201600763

Boldyrev, A. I.; Wang, L. S.
Beyond organic chemistry: aromaticity in atomic clusters
Physical Chemistry Chemical Physics, (18): 11589-11605. 2016. 10.1039/c5cp07465g

Bolotin, D. S.; Burianova, V. K.; Novikov, A. S.; Demakova, M. Y.; Pretorius, C.; Mokolokolo, P. P.; Roodt, A.; Bokach, N. A.; Suslonov, V. V.; Zhdanov, A. P.; Zhizhin, K. Y.; Kuznetsov, N. T.; Kukushkin, V. Y.
Nucleophilicity of Oximes Based upon Addition to a Nitrilium closo-Decaborate Cluster
Organometallics, (35): 3612-3623. 2016. 10.1021/acs.organomet.6b00678

Bonsaii, M.; Gholivand, K.; Abdi, K.; Valmoozi, A. A. E.; Khosravi, M.
A combined experimental and computational study on the interaction of nitrogen mustards with DNA
Medchemcomm, (7): 2003-2015. 2016. 10.1039/c6md00264a

Borca, C. H.; Arango, C. A.
Molecular Dynamics of a Water-Absorbent Nanoscale Material Based on Chitosan
Journal of Physical Chemistry B, (120): 3754-3764. 2016. 10.1021/acs.jpcb.5b11230

Borca, C. H.; Slipchenko, L. V.; Wasserman, A.
Ground-State Charge Transfer: Lithium-Benzene and the Role of Hartree-Fock Exchange
Journal of Physical Chemistry A, (120): 8190-8198. 2016. 10.1021/acs.jpca.6b09014

Borges, A.; Solomon, G. C.
An approach to develop chemical intuition for atomistic electron transport calculations using basis set rotations
Journal of Chemical Physics, (144) 2016. 10.1063/1.4950828

Borges, I.; Uhl, E.; Modesto-Costa, L.; Aquino, A. J. A.; Lischka, H.
Insight into the Excited State Electronic and Structural Properties of the Organic Photovoltaic Donor Polymer Poly(thieno 3,4-b thiophene benzodithiophene) by Means of ab Initio and Density Functional Theory
Journal of Physical Chemistry C, (120): 21818-21826. 2016. 10.1021/acs.jpcc.6b07689

Borgohain, R.; Handique, J. G.; Guha, A. K.; Pratihar, S.
A theoretical study on antioxidant activity of ferulic acid and its ester derivatives
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500280

Borin, V. A.; Matveev, S. M.; Budkina, D. S.; El-Khoury, P. Z.; Tarnovsky, A. N.

Direct photoisomerization of CH₂I₂ vs. CHBr₃ in the gas phase: a joint 50 fs experimental and multireference resonance-theoretical study
Physical Chemistry Chemical Physics, (18): 28883-28892. 2016. 10.1039/c6cp05129d

- Borosky, G. L.
Mutagenicity of heteroaromatic amines: Computational study on the influence of methyl substituents
Journal of Molecular Graphics & Modelling, (69): 92-102. 2016. 10.1016/j.jmgm.2016.08.010
- Borrman, T.; Swiderek, P.
Formation of 2-propanol in condensed molecular films of acetaldehyde following electron impact ionisation-induced proton transfer
European Physical Journal D, (70) 2016. 10.1140/epjd/e2016-70116-7
- Borthakur, B.; Silvi, B.; Dewhurst, R. D.; Phukan, A. K.
Theoretical Strategies Toward Stabilization of Singlet Remote N-Heterocyclic Carbenes
Journal of Computational Chemistry, (37): 1484-1490. 2016. 10.1002/jcc.24362
- Borthakur, R.; Prakash, R.; Nandi, P.; Ghosh, S.
Metal rich metallaboranes of group 9 transition metals
Journal of Organometallic Chemistry, (825): 1-7. 2016. 10.1016/j.jorgchem.2016.10.008
- Boserle, J.; Alonso, M.; Jambor, R.; Ruzicka, A.; Dostal, L.
Synthesis and reactivity of a germylene stabilized by a boraguanidinate ligand
RSC Advances, (6): 19377-19388. 2016. 10.1039/c6ra01187
- Boughdiri, M. A.; Boubaker, T.; Tangour, B.
Theoretical investigation of methoxide ion reaction on the 7-methyl-4,6-dinitrobenzofuroxan
Canadian Journal of Chemistry, (94): 699-703. 2016. 10.1139/cjc-2016-0034
- Boughdiri, M. A.; Tangour, B.; Boubaker, T.
Theoretical and experimental reinvestigation of methoxide ion reaction with 7-methyl 4-nitro benzofuroxan
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500309
- Boulmene, R.; Boussouf, K.; Prakash, M.; Komiha, N.; Al-Mogren, M. M.; Hochlaf, M.
AbInitio and DFT Studies on CO₂ Interacting with Znq+Imidazole (q=0, 1, 2) Complexes: Prediction of Charge Transfer through sigma- or pi-Type Models
Chemphyschem, (17): 994-1005. 2016. 10.1002/cphc.201501185
- Branzanic, A. M. V.; Lupan, A.; King, R. B.
Dimettalaborane analogues of the octaboranes of the type Cp₂M₂B₆H₁₀: structural variations with changes in the skeletal electron count
Dalton Transactions, (45): 9354-9362. 2016. 10.1039/c6dt00985a
- Brauns, M.; Muller, F.; Gulden, D.; Bose, D.; Frey, W.; Breugst, M.; Pietruszka, J.
Enantioselective Catalysts for the Synthesis of alpha-Substituted Allylboronates-An Accelerated Approach towards Isomerically Pure Homoallylic Alcohols
Angewandte Chemie-International Edition, (55): 1548-1552. 2016. 10.1002/anie.201509198
- Braunschweig, H.; Celik, M. A.; Dewhurst, R. D.; Ferkinghoff, K.; Hermann, A.; Jimenez-Halla, J. O. C.; Kramer, T.; Radacki, K.; Shang, R.; Siedler, E.; Weissenberger, F.; Werner, C.
Interactions of Isonitriles with Metal-Boron Bonds: Insertions, Coupling, Ring Formation, and Liberation of Monovalent Boron
Chemistry-a European Journal, (22): 11736-11744. 2016. 10.1002/chem.201600793
- Braunschweig, H.; Celik, M. A.; Dewhurst, R. D.; Ferkinghoff, K.; Radacki, K.; Weissenberger, F.
Boron-Metallated Borirenes and Bis(Borirenes)
Chemistry-a European Journal, (22): 8596-8602. 2016. 10.1002/chem.201600651

- Braunschweig, H.; Jimenez-Halla, J. O. C.; Radacki, K.; Shang, R.
Direct Conversion from Terminal Borylene into Terminal Phosphinidene
Angewandte Chemie-International Edition, (55): 12673-12677. 2016. 10.1002/anie.201603548
- Brea, O.; El Khatib, M.; Bendazzoli, G. L.; Evangelisti, S.; Leininger, T.; Angelici, C.
The Spin-Partitioned Total-Position Spread Tensor: An Application To Diatomic Molecules
Journal of Physical Chemistry A, (120): 5230-5238. 2016. 10.1021/acs.jpca.6b01043
- Brea, O.; Mo, O.; Yanez, M.; Alkorta, I.; Elguero, J.
On the existence of intramolecular one-electron Be-Be bonds
Chemical Communications, (52): 9656-9659. 2016. 10.1039/c6cc04350j
- Bresien, J.; Faust, K.; Hering-Junghans, C.; Rothe, J.; Schulz, A.; Villinger, A.
Synthetic strategies to bicyclic tetraphosphphanes using P-1, P-2 and P-4 building blocks
Dalton Transactions, (45): 1998-2007. 2016. 10.1039/c5dt02757h
- Bresien, J.; Ott, H.; Rosenstengel, K.; Schulz, A.; Thiele, P.; Villinger, A.
Binary Polyazides of Zinc
European Journal of Inorganic Chemistry: 5594-5609. 2016. 10.1002/ejic.201601035
- Bresien, J.; Schulz, A.; Villinger, A.
CIP(mu-PMes) (2)-A versatile reagent in phosphorus chemistry*
Phosphorus Sulfur and Silicon and the Related Elements, (191): 601-604. 2016. 10.1080/10426507.2015.1128915
- Bresien, J.; Schulz, A.; Villinger, A.
Low temperature isolation of a dinuclear silver complex of the cyclotetraphosphphane CIP(mu-PMes) (2)*
Dalton Transactions, (45): 498-501. 2016. 10.1039/c5dt03928b
- Breugst, M.; Detmar, E.; von der Heiden, D.
Origin of the Catalytic Effects of Molecular Iodine: A Computational Analysis
ACS Catalysis, (6): 3203-3212. 2016. 10.1021/acscatal.6b00447
- Brinck, T.; Carlqvist, P.; Stenlid, J. H.
Local Electron Attachment Energy and Its Use for Predicting Nucleophilic Reactions and Halogen Bonding
Journal of Physical Chemistry A, (120): 10023-10032. 2016. 10.1021/acs.jpca.6b10142
- Brugos, J.; Cabeza, J. A.; Garcia-Alvarez, P.; Kennedy, A. R.; Perez-Carreno, E.; Van der Maelen, J. F.
2-(Methylamido)pyridine-Borane: A Tripod kappa(3)-N,H,H Ligand in Trigonal Bipyramidal Rhodium(I) and Iridium(I) Complexes with an Asymmetric Coordination of Its BH₃ Group
Inorganic Chemistry, (55): 8905-8912. 2016. 10.1021/acs.inorgchem.6b01427
- Buchala, T.; Chudoba, A.; Roszak, S.
Oxidation properties of beta-substituted pyrroles
Structural Chemistry, (27): 185-189. 2016. 10.1007/s11224-015-0709-2
- Bucinsky, L.; Rohde, G. T.; Que, L.; Ozarowski, A.; Krzystek, J.; Breza, M.; Telser, J.
HFEPR and Computational Studies on the Electronic Structure of a High-Spin Oxidoiron(IV) Complex in Solution
Inorganic Chemistry, (55): 3933-3945. 2016. 10.1021/acs.inorgchem.6b00169
- Buil, M. L.; Cardo, J. J. F.; Esteruelas, M. A.; Fernandez, I.; Onate, E.
An Entry to Stable Mixed Phosphine-Osmium-NHC Polyhydrides
Inorganic Chemistry, (55): 5062-5070. 2016. 10.1021/acs.inorgchem.6b00658
- Bull, J. N.; West, C. W.; Verlet, J. R. R.
Ultrafast dynamics of formation and autodetachment of a dipole-bound state in an open-shell pi-stacked dimer anion
Chemical Science, (7): 5352-5361. 2016. 10.1039/c6sc01062h
- Bundhun, A.; Momeni, M. R.; Shakib, F. A.; Ramasami, P.; Gaspar, P. P.; Schaefer, H. F.

Toward unsaturated stannylenes Y(2)Z=Sn: and related compounds with triplet electronic ground states
RSC Advances, (6): 53749-53759. 2016. 10.1039/c6ra00492j

Burkhardt, S. E.; Petrov, V. A.; Manzo, S. M.

Computational study of the reaction mechanism of vinyl ethers with hexafluorothioacetone
Journal of Fluorine Chemistry, (191): 103-109. 2016. 10.1016/j.jfluchem.2016.09.018

Busujima, T.; Tanaka, H.

AN EFFICIENT AND CONVENIENT SYNTHESIS OF ACYL CoA: MONOACYLGLYCEROL ACYLTRANSFERASE 2 INHIBITOR, 2-2-(4-tert-BUTYLPHENYL)ETHYL -N- 4-(3-CYCLOPENTYL-PROPYL)-2-FLUOROPHENYL -1,2,3,4-TETRAHYDROISOQUINOLINE-6-SULFONAMIDE
Heterocycles, (92): 470-484. 2016. 10.3987/com-15-13387

Butera, V.; Russo, N.; Cosentino, U.; Greco, C.; Moro, G.; Pitea, D.; Sicilia, E.

Computational Insight on CO₂ Fixation to Produce Styrene Carbonate Assisted by a Single-Center Aluminum(III) Catalyst and Quaternary Ammonium Salts
Chemcatchem, (8): 1167-1175. 2016. 10.1002/cctc.201501272

Caballero-Garcia, G.; Reyes-Lezama, M.; Martinez-Otero, D.; Romero-Ortega, M.; Barroso-Flores, J.

Aromatization of pyridinylidenes into pyridines is inhibited by exocyclic delocalization. A theoretical mechanistic assessment
Tetrahedron, (72): 4194-4200. 2016. 10.1016/j.tet.2016.05.058

Cabezas, C.; Guillemin, J. C.; Endo, Y.

Fourier-transform microwave spectroscopy of a halogen substituted Criegee intermediate ClCHO
Journal of Chemical Physics, (145) 2016. 10.1063/1.4967250

Cakir, K.; Erdem, S. S.; Atalay, V. E.

ONIOM calculations on serotonin degradation by monoamine oxidase B: insight into the oxidation mechanism and covalent reversible inhibition
Organic & Biomolecular Chemistry, (14): 9239-9252. 2016. 10.1039/c6ob01175f

Calderon, L. A.; Chamorro, E.; Espinal, J. F.

Mechanisms for homogeneous and heterogeneous formation of methane during the carbon-hydrogen reaction over zigzag edge sites
Carbon, (102): 390-402. 2016. 10.1016/j.carbon.2016.02.052

Camarada, M. B.

DFT investigation of the interaction of gold nanoclusters with poly(amidoamine) PAMAM G0 dendrimer
Chemical Physics Letters, (654): 29-36. 2016. 10.1016/j.cplett.2016.05.007

Cano, J.; Lloret, F.; Julve, M.

Theoretical design of magnetic wires from acene and nanocorone derivatives
Dalton Transactions, (45): 16700-16708. 2016. 10.1039/c6dt02406h

Cao, B. B.; Du, J. Y.; Du, D. M.; Sun, H. T.; Zhu, X.; Fu, H.

Cellobiose as a model system to reveal cellulose dissolution mechanism in acetate-based ionic liquids: Density functional theory study substantiated by NMR spectra
Carbohydrate Polymers, (149): 348-356. 2016. 10.1016/j.carbpol.2016.04.128

Cao, B. B.; Liu, S. Y.; Du, D. M.; Xue, Z. M.; Fu, H.; Sun, H. T.

Experiment and DFT studies on radioiodine removal and storage mechanism by imidazolium-based ionic liquid
Journal of Molecular Graphics & Modelling, (64): 51-59. 2016. 10.1016/j.jmgm.2015.10.008

Cao, G. J.; Lu, S. J.; Xu, H. G.; Xu, X. L.; Zheng, W. J.

Structures and electronic properties of B2Si6-/0/+:anion photoelectron spectroscopy and theoretical calculations
RSC Advances, (6): 62165-62171. 2016. 10.1039/c6ra08251c

- Cao, H. Y.; Si, D. H.; Tang, Q.; Zheng, X. F.; Hao, C.
Electronic structures and solvent effects of unsymmetrical neo-confused porphyrin: DFT and TDDFT-IEPCM investigations
Computational and Theoretical Chemistry, (1081): 18-24. 2016. 10.1016/j.comptc.2016.01.012
- Cao, J.; Li, Q.; Wang, Z. X.; Gao, L. J.; Fu, F.; Fan, B.; Wang, Y.
Computational Studies on the Mo-Doped Gold Nanoclusters Au (n) Mo(n=1-10): Structures, Stabilities and Magnetic Properties
Journal of Cluster Science, (27): 993-1004. 2016. 10.1007/s10876-015-0961-z
- Cao, J. S.; Chen, F. W.
Theoretical Study on the Correlation of the Experimental Nucleophilic and Electrophilic Reaction Rates of Aromatic Compounds with the Prediction Results of Theoretical Methods
Chinese Journal of Organic Chemistry, (36): 2463-2471. 2016. 10.6023/cjoc201602026
- Cao, L. L.; Daley, E.; Johnstone, T. C.; Stephan, D. W.
Cationic aluminum hydride complexes: reactions of carbene-alane adducts with trityl-borate
Chemical Communications, (52): 5305-5307. 2016. 10.1039/c6cc01585a
- Cao, S. W.; Wang, J. R.; Tan, C. M.; Zhang, X.; Li, S.; Tian, W.; Guo, H. X.; Wang, L.; Qin, Z.
Solvent extraction of americium(III) and europium(III) with tridentate N,N-dialkyl-1,10-phenanthroline-2-amide-derived ligands: extraction, complexation and theoretical study
New Journal of Chemistry, (40): 10560-10568. 2016. 10.1039/c6nj02696f
- Cardenas-Jiron, G.; Figueroa, Y.; Kumar, N.; Seminario, J. M.
Doping Effects in the Charge Transport of Graphene-Porphyrins
Journal of Physical Chemistry C, (120): 2013-2026. 2016. 10.1021/acs.jpcc.5b08624
- Caretto, A.; Bortoluzzi, M.; Selva, M.; Perosa, A.
Dimethylcarbonate-Assisted Ring-Opening of Biobased Valerolactones with Methanol
ACS Sustainable Chemistry & Engineering, (4): 6193-6199. 2016. 10.1021/acssuschemeng.6b01863
- Carlsson, A. C. C.; Mehmeti, K.; Uhrbom, M.; Karim, A.; Bedin, M.; Puttreddy, R.; Kleinmaier, R.; Neverov, A. A.; Nekoueishahraki, B.; Grafenstein, J.; Rissanen, K.; Erdelyi, M.
Substituent Effects on the N-I-N (+) Halogen Bond
Journal of the American Chemical Society, (138): 9853-9863. 2016. 10.1021/jacs.6b03842
- Carrasco, D.; Garcia-Melchor, M.; Casares, J. A.; Espinet, P.
Dramatic mechanistic switch in Sn/Au-I group exchanges: transmetalation vs. oxidative addition
Chemical Communications, (52): 4305-4308. 2016. 10.1039/c5cc10496c
- Carrizo, E. D. S.; Fernandez, I.
The effect of the metal fragment on the aromaticity and synchronicity of the gold(I)-catalysed divinylcyclopropane-cycloheptadiene rearrangement
Physical Chemistry Chemical Physics, (18): 11677-11682. 2016. 10.1039/c5cp06523b
- Casanova, D.; Matxain, J. M.; Ugalde, J. M.
Plasmonic Resonances in the Al-13(-) Cluster: Quantification and Origin of Exciton Collectivity
Journal of Physical Chemistry C, (120): 12742-12750. 2016. 10.1021/acs.jpcc.6b03210
- Castano, J. A. G.; Romano, R. M.; Salamanca, A. R.; Amesquita, G.; Beckers, H.; Willner, H.; Della Vedova, C. O.
Vibrational spectra, conformational properties and argon matrix photochemistry of diacetyl diselenide, CH₃C(O)Se₂C(O)CH₃
Journal of Physical Organic Chemistry, (29): 636-644. 2016. 10.1002/poc.3587
- Caulkins, B. G.; Young, R. P.; Kudla, R. A.; Yang, C.; Bittbauer, T. J.; Bastin, B.; Hilario, E.; Fan, L.; Marsella, M. J.; Dunn, M. F.; Mueller, L. J.

NMR Crystallography of a Carbanionic Intermediate in Tryptophan Synthase: Chemical Structure, Tautomerization, and Reaction Specificity
Journal of the American Chemical Society, (138): 15214-15226. 2016. 10.1021/jacs.6b08937

Cekli, S.; Winkel, R. W.; Schanze, K. S.
Effect of Oligomer Length on Photophysical Properties of Platinum Acetylide Donor-Acceptor-Donor Oligomers
Journal of Physical Chemistry A, (120): 5512-5521. 2016. 10.1021/acs.jpca.6b03977

Celik, S.; Ozel, A. E.; Akyuz, S.
Comparative study of antitumor active cyclo(Gly-Leu) dipeptide: A computational and molecular modeling study
Vibrational Spectroscopy, (83): 57-69. 2016. 10.1016/j.vibspec.2016.01.007

Ceylan, U.; Haciyyusufoglu, M. E.; Yalcinc, S. P.; Sonmez, M.; Aygun, M.
Synthesis, molecular structure and spectroscopic characterization of (E)-1-((2-hydroxynaphthalen-1-yl)methyleneamino)-5-(4-methoxybenzoyl)-4-(4-methoxyphenyl) pyrimidine-2(1H)-one with experimental techniques and theoretical calculations
Journal of Molecular Structure, (1109): 209-219. 2016. 10.1016/j.molstruc.2016.01.011

Chaabene, M.; Khatyr, A.; Knorr, M.; Askri, M.; Rousselain, Y.; Kubicki, M. M.
Bis{(4-methylthio)phenylthio}methane as assembling ligand for the construction of Cu(I) and Hg(II) coordination polymers. Crystal structures and topological (AIM) analysis of the bonding
Inorganica Chimica Acta, (451): 177-186. 2016. 10.1016/j.ica.2016.07.023

Chafaa, F.; Hellel, D.; Nacereddine, A. K.; Djerourou, A.
A theoretical study of the mechanism and selectivity of the intramolecular 1,3-dipolar cycloaddition reaction of the nitrone-alkene derived from 2-allylthiobenzaldehyde for the synthesis of tricyclic isoxazolidines
Tetrahedron Letters, (57): 67-70. 2016. 10.1016/j.tetlet.2015.11.069

Chafaa, F.; Hellel, D.; Nacereddine, A. K.; Djerourou, A.
A theoretical study of the regio- and stereoselectivities of non-polar 1,3-dipolar cycloaddition reaction between C-diethoxyphosphoryl-N-methylnitrone and N-(2-fluorophenyl)acrylamide
Molecular Physics, (114): 663-670. 2016. 10.1080/00268976.2015.1111458

Chahkandi, M.
V-51 NMR, O-17 NMR, and UV-Vis computational studies of new VBPO functional models: Bromide oxidation reaction
Polyhedron, (109): 92-98. 2016. 10.1016/j.poly.2016.02.006

Chahkandi, M.; Khoshbakht, B. M.; Mirzaei, M.
A theoretical study of intramolecular H-bonding and metal-ligand interactions in some complexes with bicyclic guanidine ligands
Computational and Theoretical Chemistry, (1095): 36-43. 2016. 10.1016/j.comptc.2016.09.014

Chain, F. E.; Ladetto, M. F.; Grau, A.; Catalan, C. A. N.; Brandan, S. A.
*Structural, electronic, topological and vibrational properties of a series of N-benzylamides derived from Maca (*Lepidium meyenii*) combining spectroscopic studies with ONION calculations*
Journal of Molecular Structure, (1105): 403-414. 2016. 10.1016/j.molstruc.2015.10.082

Chakraborty, D.; Chattaraj, P. K.
Possible sequestration of polar gas molecules by superhalogen supported aluminum nitride nanoflakes
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3153-3

Chakraborty, R.; Ghosh, D.
The effect of sequence on the ionization of guanine in DNA
Physical Chemistry Chemical Physics, (18): 6526-6533. 2016. 10.1039/c5cp07804k

Chakraborty, S.; Purkayastha, D. D.; Das, G.; Bhattacharjee, C. R.; Mondal, P.; Prasad, S. K.; Rao, D. S. S.
Photoluminescent tetrahedral d(10)-metal Schiff base complexes exhibiting highly ordered mesomorphism
Polyhedron, (105): 150-158. 2016. 10.1016/j.poly.2015.11.053

- Chalabala, J.; Slavicek, P.
Nonadiabatic dynamics of floppy hydrogen bonded complexes: the case of the ionized ammonia dimer
Physical Chemistry Chemical Physics, (18): 20422-20432. 2016. 10.1039/c6cp02714h
- Chalmers, B. A.; Meigh, C. B. E.; Nejman, P. S.; Buhl, M.; Lebl, T.; Woollins, J. D.; Slawin, A. M. Z.; Kilian, P.
Geminally Substituted Tris(acenaphthyl) and Bis(acenaphthyl) Arsines, Stibines, and Bismuthine: A Structural and Nuclear Magnetic Resonance Investigation
Inorganic Chemistry, (55): 7117-7125. 2016. 10.1021/acs.inorgchem.6b01079
- Chambers, G. M.; Huynh, M. T.; Li, Y. L.; Hammes-Schiffer, S.; Rauchfuss, T. B.; Reijerse, E.; Lubitz, W.
*Models of the Ni-L and Ni-*S*(*a*) States of the NiFe -Hydrogenase Active Site*
Inorganic Chemistry, (55): 419-431. 2016. 10.1021/acs.inorgchem.5b01662
- Charanya, C.; Sampathkrishnan, S.; Balamurugan, N.
Natural Bond Orbitals (NBO), Natural Population Analysis, Mulliken Analysis of Atomic Charges of L-Alaninium Oxalate Spectroscopy and Spectral Analysis, (36): 2721-2724. 2016. 10.3964/j.issn.1000-0593(2016)08-2721-04
- Charboneau, D. J.; Balcells, D.; Hazari, N.; Lant, H. M. C.; Mayer, J. M.; Melvin, P. R.; Mercado, B. Q.; Morris, W. D.; Repisky, M.; Suh, H. W.
Dinitrogen-Facilitated Reversible Formation of a Si-H Bond in a Pincer-Supported Ni Complex
Organometallics, (35): 3154-3162. 2016. 10.1021/acs.organomet.6b00514
- Charette, B. J.; Ritch, J. S.
A Selenium-Containing Diarylamido Pincer Ligand: Synthesis and Coordination Chemistry with Group 10 Metals
Inorganic Chemistry, (55): 6344-6350. 2016. 10.1021/acs.inorgchem.6b01203
- Chatterjee, A.; Eliasson, S. H. H.; Tornroos, K. W.; Jensen, V. R.
Palladium Precatalysts for Decarbonylative Dehydration of Fatty Acids to Linear Alpha Olefins
ACS Catalysis, (6): 7784-7789. 2016. 10.1021/acscatal.6b02460
- Chatterjee, S.; Wang, F.
How different is pyrimidine as a core component of DNA base from its diazine isomers: A DFT study?
International Journal of Quantum Chemistry, (116): 1836-1845. 2016. 10.1002/qua.25229
- Chatturgoon, T.; Akerman, M. P.
X-ray and DFT-calculated structures of bis N-(quinolin-8-yl)benzamidato-kappa N-2,N' copper(II)
Acta Crystallographica Section C-Structural Chemistry, (72): 234-. 2016. 10.1107/s2053229616003120
- Chauvin, J. P. R.; Haidasz, E. A.; Griesser, M.; Pratt, D. A.
Polysulfide-1-oxides react with peroxy radicals as quickly as hindered phenolic antioxidants and do so by a surprising concerted homolytic substitution
Chemical Science, (7): 6347-6356. 2016. 10.1039/c6sc01434h
- Chen, H.; Wang, W. Y.; Wang, L.; Zhu, C. L.; Fang, X. Y.; Qiu, Y. Q.
Ion-pi interaction in impacting the nonlinear optical properties of ion-buckybowl complexes
Journal of Molecular Graphics & Modelling, (64): 139-146. 2016. 10.1016/j.jmgm.2016.01.008
- Chen, J.; Zhang, H. Y.; Liu, X. H.; Yuan, C. Q.; Jia, M. Y.; Luo, Z. X.; Yao, J. N.
Charge-transfer interactions between TCNQ and silver clusters Ag-20 and Ag-13
Physical Chemistry Chemical Physics, (18): 7190-7196. 2016. 10.1039/c5cp06892d
- Chen, K. X.; Xie, H. Y.; Mao, J. Y.; Jiang, K. Z.
Structure-performance landscape of N-alkoxyphthalimides as organocatalysts in aerobic oxidation
Journal of Catalysis, (344): 229-235. 2016. 10.1016/j.jcat.2016.09.015
- Chen, M. J.; Fu, Y. W.; Qi, J. S.

*The Effects of Acceptor Moiety and Donor-to-Acceptor Ratio on the Geometries and Electronic Properties of Thieno 3,2-*b* thiophene-based Donor-Acceptor Alternating Copolymers*
Acta Polymerica Sinica: 31-39. 2016.

Chen, P. E.; McNeely, J.; Lum, J. S.; Gardner, E. J.; Phillips, V.; Golen, J. A.; Rheingold, A. L.; Doerrer, L. H.
LCu(mu-X)(2)CuL compounds: An induced cuprophilic interaction
Polyhedron, (116): 204-215. 2016. 10.1016/j.poly.2016.05.033

Chen, P. Y.; Zhang, L.; Zhu, S. G.; Cheng, G. B.
Intermolecular Interactions, Thermodynamic Properties, Detonation Performance, and Sensitivity of TNT/CL-20 Cocrystal Explosive
Chinese Journal of Structural Chemistry, (35): 246-256. 2016.

Chen, Q.; Li, H. R.; Tian, W. J.; Lu, H. G.; Zhai, H. J.; Li, S. D.
Endohedral charge-transfer complex Ca@B-37(-): stabilization of a B-37(3-) borospherene trianion by metal-encapsulation
Physical Chemistry Chemical Physics, (18): 14186-14190. 2016. 10.1039/c6cp02369j

Chen, S.; Li, Y.; Yang, D. W.; Luo, L.; Qu, J. P.; Luo, Y.
Studies on the electronic structure of thiolate-bridged diiron complexes and their single-electron reduction reactions
Chemical Physics Letters, (660): 117-122. 2016. 10.1016/j.cplett.2016.08.011

Chen, S.; Luo, L.; Li, Y.; Yang, D. W.; Qu, J. P.; Luo, Y.
Electronic Structure of Thiolate-bridged Diiron Complexes and a Single-electron Oxidation Reaction: A Combination of Experimental and Computational Studies
Chinese Journal of Chemistry, (34): 919-924. 2016. 10.1002/cjoc.201600262

Chen, X. H.; Yuan, L.; Leng, X. Q.; Jin, R.; Du, Q.; Feng, H.; Xie, Y. M.; King, R. B.; Schaefer, H. F.
Effect of metal complexation on the equilibrium between methylphosphepine and methylphosphanorcaradiene and their benzo analogues
New Journal of Chemistry, (40): 7804-7813. 2016. 10.1039/c6nj01481j

Chen, X. H.; Yuan, L.; Ren, G. M.; Xi, Q.; Jin, R.; Du, Q.; Feng, H.; Xie, Y. M.; King, R. B.
Binuclear phospholyl iron carbonyls: The limited role of the phosphorus atom in metal complexation
Inorganica Chimica Acta, (445): 79-86. 2016. 10.1016/j.ica.2016.02.017

Chen, X. H.; Yuan, L.; Wan, X.; Jin, R.; Du, Q.; Feng, H.; Xie, Y. M.; King, R. B.
1,3-Diphosphacyclobutadiene as a ligand in binuclear manganese carbonyl derivatives: Role of the ring phosphorus atoms
Inorganica Chimica Acta, (446): 116-123. 2016. 10.1016/j.ica.2016.02.055

Chen, Y. L.; Wu, D. Y.; Tian, Z. Q.
Theoretical Investigation on the Substituent Effect of Halogen Atoms at the C-8 Position of Adenine: Relative Stability, Vibrational Frequencies, and Raman Spectra of Tautomers
Journal of Physical Chemistry A, (120): 4049-4058. 2016. 10.1021/acs.jpca.6b03604

Chen, Y. W.; Sun, X.; Wu, N. J.; Li, J. B.; Jin, S. N.; Zhong, Y. L.; Liu, Z. R.; Rogachev, A.; Chong, H. S.
Synthetic and theoretical investigation on the one-pot halogenation of beta-amino alcohols and nucleophilic ring opening of aziridinium ions
Organic & Biomolecular Chemistry, (14): 920-939. 2016. 10.1039/c5ob01692d

Chen, Z. J.; Tian, Z. Q.; Kallio, K.; Oleson, A. L.; Ji, A.; Borchardt, D.; Jiang, D. E.; Remington, S. J.; Ai, H. W.
The N-B Interaction through a Water Bridge: Understanding the Chemoselectivity of a Fluorescent Protein Based Probe for Peroxynitrite
Journal of the American Chemical Society, (138): 4900-4907. 2016. 10.1021/jacs.6b01285

Chen, Z. Q.; Wang, G. M.; Xu, Z. J.; Wang, J. A.; Yu, Y. Q.; Cai, T. T.; Shao, Q.; Shi, J. Y.; Zhu, W. L.
How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?

Journal of Physical Chemistry B, (120): 8784-8793. 2016. 10.1021/acs.jpcb.6b05027

Cheng, Q. Y.; Teng, Q.; Marchitti, S. A.; Dillingham, C. M.; Kenneke, J. F.
An Integrated Experimental and Computational Approach for Characterizing the Kinetics and Mechanism of Triadimefon Racemization Chirality, (28): 633-641. 2016. 10.1002/chir.22622

Cheng, S. S.; Shi, Y.; Ma, X. N.; Xing, D. X.; Liu, L. D.; Liu, Y.; Zhao, Y. X.; Sui, Q. C.; Tan, X. J.
Synthesis, crystal structure, spectroscopic properties and potential anti-cancerous activities of four unsaturated bis-norcantharimides
Journal of Molecular Structure, (1115): 228-240. 2016. 10.1016/j.molstruc.2016.02.093

Cheng, Y. M.; Wang, X. Y.; Li, W. W.; Chang, D.
DFT study on the effects of beta-cyclodextrin in synthesis of 2-phenylbenzimidazole via benzaldehyde and o-phenylenediamine
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3161-3

Cheng, Z. P.; Wu, Q. Y.; Liu, Y. H.; Lan, J. H.; Wang, C. Z.; Chai, Z. F.; Shi, W. Q.
The redox mechanism of Np-VI with hydrazine: a DFT study
RSC Advances, (6): 109045-109053. 2016. 10.1039/c6ra13339h

Chermahini, A. N.; Chermahini, Z. J.
Comparing the ion affinity of two ionophores: Theoretical study of alkali earth metal ion-nano tubular cyclic peptide complexes
Journal of Molecular Liquids, (214): 101-110. 2016. 10.1016/j.molliq.2015.12.024

Chermahini, Z. J.; Chermahini, A. N.
Theoretical study of microhydrated cyclo(L-pro)(4)-alkali cation complexes
Computational and Theoretical Chemistry, (1078): 37-46. 2016. 10.1016/j.comptc.2015.12.020

Chi, W. J.; Guo, Y. Y.; Li, Q. S.; Li, Z. S.
Substituent effects on the properties related to detonation performance and stability for pentaprismane derivatives
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1885-x

Cho, D.; Ko, K. C.; Lee, J. Y.
Quantum chemical approaches for controlling and evaluating intramolecular magnetic interactions in organic diradicals
International Journal of Quantum Chemistry, (116): 578-597. 2016. 10.1002/qua.25060

Cho, H. G.; Andrews, L.
Infrared Spectra and Density Functional Calculations for Singlet CH₂=SiX₂ and Triplet HC-SiX₃ and XC-SiX₃ Intermediates in Reactions of Laser-Ablated Silicon Atoms with Di-, Tri-, and Tetrahalomethanes
Inorganic Chemistry, (55): 2819-2829. 2016. 10.1021/acs.inorgchem.5b02610

Cho, H. G.; Andrews, L.
Infrared Spectra and DFT Calculations of Planar and Bridged Methyldene Intermediates in Reactions of Laser-Ablated Yttrium and Lanthanum Atoms with Di-, Tri-, and Tetrahalomethanes
European Journal of Inorganic Chemistry: 380-392. 2016. 10.1002/ejic.201501216

Cho, H. G.; Andrews, L.
Infrared Spectra and Structures of SiH₂-(CH₂)₂ and CH₂CH-SiH₃ Intermediates Prepared in Reactions of Laser-ablated Silicon Atoms with Ethane
Bulletin of the Korean Chemical Society, (37): 415-417. 2016. 10.1002/bkcs.10690

Chohan, T. A.; Qian, H. Y.; Pan, Y. L.; Chen, J. Z.
Molecular simulation studies on the binding selectivity of 2-anilino-4-(thiazol-5-yl)-pyrimidines in complexes with CDK2 and CDK7
Molecular Biosystems, (12): 145-161. 2016. 10.1039/c5mb00630a

- Choi, C.; Yoo, H. W.; Goh, E. M.; Cho, S. G.; Jung, Y.
Ti(N-5)(4) as a Potential Nitrogen-Rich Stable High-Energy Density Material
Journal of Physical Chemistry A, (120): 4249-4255. 2016. 10.1021/acs.jpca.6b04226
- Choony, N.; Rowe, G. T.; Choony, C. D.; Earhart, L. S.; Fulmer, J. M.; Johnson, D.; Loveless, T. M.
The Use and Thermodynamic Origin of the Trityl Buttress Effect in Intramolecular Diels-Alder Cycloaddition Reactions
Current Organic Synthesis, (13): 617-622. 2016. 10.2174/1570179413666151218203401
- Chowdhury, M. A. H.; Rahman, M. S.; Islam, M. R.; Rajbangshi, S.; Ghosh, S.; Hogarth, G.; Tocher, D. A.; Yang, L.; Richmond, M. G.; Kabir, S. E.
Iron carbonyl complexes bearing phenazine and acridine ligands: X-ray structures of Fe(CO)(3)(eta(4)-C12H8N2), Fe(CO)(2){P(OMe)(3)}(eta(4)-C12H8N2), Fe(CO)(2)(PPh3) (eta(4)-C13H9N), and Fe(CO)(2)(kappa(1)-dppm) (eta(4)-C12H8N2)
Journal of Organometallic Chemistry, (805): 34-41. 2016. 10.1016/j.jorgchem.2015.12.023
- Christensen, A. S.; Kubar, T.; Cui, Q.; Elstner, M.
Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications
Chemical Reviews, (116): 5301-5337. 2016. 10.1021/acs.chemrev.5b00584
- Chu, G. M.; Guerrero-Martinez, A.; de Arellano, C. R.; Fernandez, I.; Sierra, M. A.
Remote Control by pi-Conjugation of the Emissive Properties of Fischer Carbene-BODIPY Dyads
Inorganic Chemistry, (55): 2737-2747. 2016. 10.1021/acs.inorgchem.5b02448
- Chu, T.; Vyboishchikov, S. F.; Gabidullin, B.; Nikonov, G. I.
Oxidative Cleavage of C=S and P=S Bonds at an Al-I Center: Preparation of Terminally Bound Aluminum Sulfides
Angewandte Chemie-International Edition, (55): 13306-13311. 2016. 10.1002/anie.201607735
- Chung, H. T.; Choe, Y. K.; Martinez, U.; Dumont, J. H.; Mohanty, A.; Bae, C.; Matanovic, I.; Kim, Y. S.
Effect of Organic Cations on Hydrogen Oxidation Reaction of Carbon Supported Platinum
Journal of the Electrochemical Society, (163): F1503-F1509. 2016. 10.1149/2.0511614jes
- Ci, C. G.; Liu, H. S.; Yan, L. K.; Su, Z. M.
Mechanistic Investigation into Olefin Epoxidation with H2O2 Catalyzed by Aqua-Coordinated Sandwich-Type Polyoxometalates: Role of the Noble Metal and Active Oxygen Position
Chemistryopen, (5): 470-476. 2016. 10.1002/open.201600064
- Ciancaleoni, G.; Arca, M.; Caramori, G. F.; Frenking, G.; Schneider, F. S. S.; Lippolis, V.
Bonding Analysis in Homo- and Hetero-Trihalide Species: A Charge Displacement Study
European Journal of Inorganic Chemistry: 3804-3812. 2016. 10.1002/ejic.201600471
- Cimino, P.; Raucci, U.; Donati, G.; Chiariello, M. G.; Schiazza, M.; Coppola, F.; Rega, N.
On the different strength of photoacids
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1879-8
- Cindric, M.; Pavlovic, G.; Pajic, D.; Zadro, K.; Cincic, D.; Hrenar, T.; Leksic, E.; Prieto, A. B. P.; Lazic, P.; Jung, D. S.
Correlation between structural, physical and chemical properties of three new tetrานuclear Ni-II clusters
New Journal of Chemistry, (40): 6604-6614. 2016. 10.1039/c6nj00287k
- Cochrane, B.; Naumkin, F. Y.
Reshaping and linking of molecules in ion-pair traps
Chemical Physics Letters, (643): 137-141. 2016. 10.1016/j.cplett.2015.11.034
- Cole, D. J.; Hine, N. D. M.
Applications of large-scale density functional theory in biology
Journal of Physics-Condensed Matter, (28) 2016. 10.1088/0953-8984/28/39/393001
- Conley, M. P.; Lapadula, G.; Sanders, K.; Gajan, D.; Lesage, A.; del Rosa, I.; Maron, L.; Lukens, W. W.; Coperet, C.; Andersen, R. A.

The Nature of Secondary Interactions at Electrophilic Metal Sites of Molecular and Silica-Supported Organolutetium Complexes from Solid-State NMR Spectroscopy
Journal of the American Chemical Society, (138): 3831-3843. 2016. 10.1021/jacs.6b00071

Cooper, D. L.; Ponec, R.; Kohout, M.
New insights from domain-averaged Fermi holes and bond order analysis into the bonding conundrum in C-2
Molecular Physics, (114): 1270-1284. 2016. 10.1080/00268976.2015.1112925

Cormanich, R. A.; Rittner, R.; O'Hagan, D.; Buhl, M.
Inter- and Intramolecular CF center dot center dot center dot C=O Interactions on Aliphatic and Cyclohexane Carbonyl Derivatives
Journal of Computational Chemistry, (37): 25-33. 2016. 10.1002/jcc.23918

Corne, V.; Sarotti, A. M.; de Arellano, C. R.; Spanevello, R. A.; Suarez, A. G.
Experimental and theoretical insights in the alkene-arene intramolecular pi-stacking interaction
Beilstein Journal of Organic Chemistry, (12): 1616-1623. 2016. 10.3762/bjoc.12.158

Correra, T. C.; Fernandes, A. S.; Riveros, J. M.
Dynamic/Thermochemical Balance Drives Unusual Alkyl/F Exchange Reactions in Siloxides and Analogs
Journal of Physical Chemistry A, (120): 1644-1651. 2016. 10.1021/acs.jpca.6b00390

Cortes-Arriagada, D.
Expanding the environmental applications of metal (Al, Ti, Mn, Fe) doped graphene: adsorption and removal of 1,4-dioxane
Physical Chemistry Chemical Physics, (18): 32281-32292. 2016. 10.1039/c6cp07311e

Cortes-Arriagada, D.; Toro-Labbe, A.
Aluminum and iron doped graphene for adsorption of methylated arsenic pollutants
Applied Surface Science, (386): 84-95. 2016. 10.1016/j.apsusc.2016.05.154

Cortes-Arriagada, D.; Toro-Labbe, A.
A theoretical investigation of the removal of methylated arsenic pollutants with silicon doped graphene
RSC Advances, (6): 28500-28511. 2016. 10.1039/c6ra03813a

Costa, R. A.; Pinheiro, M. L. B.; de Oliveira, K. M. T.; Barison, A.; Salome, K. S.; Iank, J. R.; da Silva, N. G.; Cabral, T. S.; Costa, E. V.
Structural, Vibrational, and Electronic Properties of the Glucoalkaloid Strictosidine: A Combined Experimental and Theoretical Study
Journal of Chemistry, 2016. 10.1155/2016/1752429

Couce-Rios, A.; Lledos, A.; Ujaque, G.
The Origin of Anti-Markovnikov Regioselectivity in Alkene Hydroamination Reactions Catalyzed by Rh(DPEphos) (+)
Chemistry-a European Journal, (22): 9311-9320. 2016. 10.1002/chem.201504645

Cruz-Olvera, D.; Geudtner, G.; Calaminici, P.
Molecular graphs of Mo_{2n}C_n (n=1-10) clusters
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-2003-9

Csordas, B.; Nagy, A.; Harmat, V.; Zsoldos-Mady, V.; Leveles, I.; Pinter, I.; Farkas, V.; Perczel, A.
Origin of problems related to Staudinger reduction in carbopeptoid syntheses
Amino Acids, (48): 2619-2633. 2016. 10.1007/s00726-016-2289-x

Cuadro, W. J.; Ensuncho, A. E.; Robles, J. R.
THEORETICAL CHARACTERIZATION AND DESIGN OF EFFICIENT PHOTOACTIVE MATERIALS BASED ON NAPHTHOPYRROLE AND NAPHTHOTHIOPHENONE DERIVATIVES AIMED TOWARDS ORGANIC SOLAR CELLS
Quimica Nova, (39): 853-858. 2016. 10.5935/0100-4042.20160101

Cui, J. H.; Yu, Z. C.; Lau, D.
Effect of Acetyl Group on Mechanical Properties of Chitin/Chitosan Nanocrystal: A Molecular Dynamics

Cui, Q.

Perspective: Quantum mechanical methods in biochemistry and biophysics

Journal of Chemical Physics, (145) 2016. 10.1063/1.4964410

Cui, Y. L.; Li, Y. F.; Dai, Y. M.; Verpoort, F.; Song, P.; Xia, L. X.

Detailed theoretical investigation of excited-state intramolecular proton transfer mechanism of a new chromophore II
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (154): 130-134. 2016.

10.1016/j.saa.2015.10.038

Cui, Z. H.; Attah, I. K.; Platt, S. P.; Aziz, S. G.; Kertesz, M.; El-Shall, M. S.

*Xe-bearing hydrocarbon ions: Observation of Xe.acetylene(+center dot) and Xe.benzene(+center dot) radical cations
and calculations of their ground state structures*

Chemical Physics Letters, (649): 8-14. 2016. 10.1016/j.cplett.2016.02.020

Cui, Z. H.; Yang, W. S.; Zhao, L. L.; Ding, Y. H.; Frenking, G.

Unusually Short Be-Be Distances with and without a Bond in Be2F2 and in the Molecular Discuses Be2B8 and Be2B7
Angewandte Chemie-International Edition, (55): 7841-7846. 2016. 10.1002/anie.201601890

Cukrowski, I.; Mangondo, P.

*Interacting quantum fragments-rooted preorganized-interacting fragments attributed relative molecular stability of
the Be-II complexes of nitrilotriacetic acid and nitrilotri-3-propionic acid*

Journal of Computational Chemistry, (37): 1373-1387. 2016. 10.1002/jcc.24346

Cukrowski, I.; Sagan, F.; Mitoraj, M. P.

On the Stability of Cis- and Trans-2-Butene Isomers. An Insight Based on the FAMSEC, IQA, and ETS-NOCV Schemes
Journal of Computational Chemistry, (37): 2783-2798. 2016. 10.1002/jcc.24504

Cysewski, P.

*Heat of formation distributions of components involved in bi-component cocrystals and simple binary eutectic
mixtures*

New Journal of Chemistry, (40): 187-194. 2016. 10.1039/c5nj02013a

Czerwinska, I.; Far, J.; Kune, C.; Larriba-Andaluz, C.; Delaude, L.; De Pauw, E.

*Structural analysis of ruthenium-arene complexes using ion mobility mass spectrometry, collision-induced dissociation,
and DFT*

Dalton Transactions, (45): 6361-6370. 2016. 10.1039/c6dt00080k

Cznotka, E.; Jeschke, S.; Wiemhofer, H. D.

*Characterization of semi-interpenetrating polymer electrolytes containing poly(vinylidene fluoride-co-
hexafluoropropylene) and ether-modified polysiloxane*
Solid State Ionics, (289): 35-47. 2016. 10.1016/j.ssi.2016.02.016

Da Silva, A. C. H.; Da Silva, J. L. F.; Franco, D. W.

Nitroxyl as a ligand in ruthenium tetraammine systems: a density functional theory study
Dalton Transactions, (45): 4907-4915. 2016. 10.1039/c5dt03706a

da Silva, M. B.; dos Santos, R. C. R.; da Cunha, A. M.; Valentini, A.; Pessoa, O. D. L.; Caetano, E. W. S.; Freire, V. N.

*Structural, Electronic, and Optical Properties of Bulk Boric Acid 2A and 3T Polymorphs: Experiment and Density
Functional Theory Calculations*
Crystal Growth & Design, (16): 6631-6640. 2016. 10.1021/acs.cgd.6b01297

da Silva, M. J. V.; Silva, R. G. M.; Melo, U. Z.; Goncalves, D. S.; Back, D. F.; Moura, S.; Pontes, R. M.; Basso, E. A.; Gauze, G. F.; Rosa, F. A.

*Theoretical and experimental investigation of the polyelectrophilic beta-enamino diketone: straightforward and highly
regioselective synthesis of 1,4,5-trisubstituted pyrazoles and pyrazolo 3,4-d pyridazinones*
RSC Advances, (6): 290-302. 2016. 10.1039/c5ra12968k

- Dadrass, A.; Rahchamani, H.
SYNTHESIS OF ORGANOPHOSPHORUS COMPLEXES AND STRUCTURAL CHARATERIZATION OF TWO DIMERIC TRIPHENYLPHOSPHINNE COMPLEXES OF MERCURY(II) IONS FROM DIMERIC COMPLEXES OF 4-METHYLBENZOYL METHYLENETRI-P-TOLYLPHOSPHINE MERCURY(II) HALIDES
Journal of the Chilean Chemical Society, (61): 2968-2972. 2016.
- Dadsetani, M.; Abdolmaleki, A.; Zabardasti, A.
Theoretical study of optical activity of 1:1 hydrogen bond complexes of water with S-warfarin
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (168): 180-189. 2016.
10.1016/j.saa.2016.06.004
- Dai, C. Q.; Yang, Y.; Fisher, A.; Liu, Z. P.; Cheng, D. J.
Interaction of CO₂ with metal cluster-functionalized ionic liquids
Journal of CO₂ Utilization, (16): 257-263. 2016. 10.1016/j.jcou.2016.08.004
- Dai, Z. Q.; Liu, J. B.; Tang, S. S.; Wang, Y.; Li, B.; Jin, R. F.
Theoretical design and selectivity researches on the enrofloxacin imprinted polymer
Structural Chemistry, (27): 1135-1142. 2016. 10.1007/s11224-015-0735-0
- Damon, P. L.; Wu, G.; Kaltsoyannis, N.; Hayton, T. W.
Formation of a Ce(IV) Oxo Complex via Inner Sphere Nitrate Reduction
Journal of the American Chemical Society, (138): 12743-12746. 2016. 10.1021/jacs.6b07932
- Dangat, Y.; Rizvi, M. A.; Pandey, P.; Vanka, K.
Exploring activity differences between the hydroformylation catalysts: Insights from theory
Journal of Organometallic Chemistry, (801): 30-41. 2016. 10.1016/j.jorgchem.2015.10.015
- Dangat, Y.; Vanka, K.
Exploring the reducing role of boron: added insights from theory
Dalton Transactions, (45): 5978-5988. 2016. 10.1039/c5dt03799a
- Darweesh, A. F.; Mansour, A. M.; Elwahy, A. H. M.
Novel bis(benzothiazole-oxime)-based Pd(II)-complex: synthesis, characterization, quantum chemical calculations, and catalytic significance in Suzuki-Miyaura and Heck-Mizoroki cross coupling reactions
Monatshefte fur Chemie, (147): 1197-1205. 2016. 10.1007/s00706-015-1633-2
- Das, A. K.; Solomon, R. V.; Hofmann, F.; Meuwly, M.
Inner-Shell Water Rearrangement Following Photoexcitation of Tris(2,2'-bipyridine)iron(II)
Journal of Physical Chemistry B, (120): 206-216. 2016. 10.1021/acs.jpcb.5b10980
- Daschakraborty, S.; Kiefer, P. M.; Miller, Y.; Motro, Y.; Pines, D.; Pines, E.; Hynes, J. T.
Reaction Mechanism for Direct Proton Transfer from Carbonic Acid to a Strong Base in Aqueous Solution I: Acid and Base Coordinate and Charge Dynamics
Journal of Physical Chemistry B, (120): 2271-2280. 2016. 10.1021/acs.jpcb.5b12742
- Dawoud, J. N.
Substitution effects on interaction forces in Na+center dot C₄H₄O complexes. Computational study
Computational and Theoretical Chemistry, (1090): 234-244. 2016. 10.1016/j.comptc.2016.06.027
- de Aguiar, S.; Stoger, B.; Pittenauer, E.; Allmaier, G.; Veiros, L. F.; Kirchner, K.
Arene C-H Bond Coordination versus C-H Bond Cleavage in Low-Valent Group 6 Carbonyl Pincer Complexes
Organometallics, (35): 3032-3039. 2016. 10.1021/acs.organomet.6b00563
- de Almeida, K. J.; Silva, T. C.; Neto, J. L.; Rocha, M. V. J.; Ramalho, T. C.; de Miranda, M. N.; Duarte, H. A.
Methane C-H bond activation by niobium oxides: Theoretical analyses of the bonding and reactivity properties of Nbo(m)(n+) (m=1, 2; n=0, 1, 2)
Journal of Organometallic Chemistry, (802): 49-59. 2016. 10.1016/j.jorgchem.2015.11.015

- Deb, D. K.; Sarkar, B.
Impact of deformation energy on the hydrogen bonding interactions in gas phase 3-X catechol center dot center dot center H₂O complexes (X = H, F, Cl, Br): The effect of approach of a water molecule
Chemical Physics, (472): 95-104. 2016. 10.1016/j.chemphys.2016.03.003
- DeBackere, J. R.; Bortolus, M. R.; Schrobilgen, G. J.
Synthesis and Characterization of XeO₂(2+) in the Adduct-Cation Salt, CH₃CN- - -XeO₂- - -NCCH₃AsF₆(2)
Angewandte Chemie-International Edition, (55): 11917-11920. 2016. 10.1002/anie.201606851
- Debnath, T.; Ash, T.; Banu, T.; Das, A. K.
Investigation of agostic interaction through NBO analysis and its impact on beta-hydride elimination and dehydrogenation: a DFT approach
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1939-0
- Debnath, T.; Saha, J. K.; Banu, T.; Ash, T.; Das, A. K.
Structural and thermodynamic aspects of Li-n@C-x endohedral metallofullerenes: a DFT approach
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1919-4
- Decken, A.; Greer, S.; Grein, F.; Mailman, A.; Mueller, B.; Paulose, T. A. P.; Passmore, J.; Rautiainen, J. M.; Richardson, S. A.; Schriver, M. J.; Whidden, T. K.
Absorption of SO₂(g) by TDAE O₂SSO₂(s) to Give TDAE O₂SS(O)(2)SO₂(s): Related Reactions of NR₄(2) O₂SSO₂(s) (R = CH₃, C₂H₅)
Inorganic Chemistry, (55): 5999-6009. 2016. 10.1021/acs.inorgchem.6b00488
- Deepak, R.; Sankararamakrishnan, R.
N-H center dot center dot center dot N Hydrogen Bonds Involving Histidine Imidazole Nitrogen Atoms: A New Structural Role for Histidine Residues in Proteins
Biochemistry, (55): 3774-3783. 2016. 10.1021/acs.biochem.6b00253
- Deepak, R.; Sankararamakrishnan, R.
Unconventional N-H center dot center dot center dot N Hydrogen Bonds Involving Proline Backbone Nitrogen in Protein Structures
Biophysical Journal, (110): 1967-1979. 2016. 10.1016/j.bpj.2016.03.034
- Del Bene, J. E.; Alkorta, I.; Elguero, J.
Anionic complexes of F- and Cl- with substituted methanes: Hydrogen, halogen, and tetrel bonds
Chemical Physics Letters, (655): 115-119. 2016. 10.1016/j.cplett.2016.05.030
- Del Bene, J. E.; Alkorta, I.; Elguero, J.
B4H₄ and B-4(CH₃)(4) as Unique Electron Donors in Hydrogen-Bonded and Halogen-Bonded Complexes
Journal of Physical Chemistry A, (120): 5745-5751. 2016. 10.1021/acs.jpca.6b05367
- Del Bene, J. E.; Alkorta, I.; Elguero, J.
Properties of cationic pnicogen-bonded complexes F_{4-n}H_nP+:N-base with H-P center dot center dot center dot N linear and n=1-4
Molecular Physics, (114): 102-117. 2016. 10.1080/00268976.2015.1086835
- Del Bene, J. E.; Alkorta, I.; Elguero, J.
Using (FH)(2) and (FH)(3) to Bridge the sigma-Hole and the Lone Pair at P in Complexes with H₂XP, for X = CH₃, OH, H, CCH, F, Cl, NC, and CN
Chemphyschem, (17): 1475-1485. 2016. 10.1002/cphc.201600048
- Del Rosal, I.; Yahia, A.; Maron, L.
Effects of the Grafting of Lanthanum Complexes on a Silica Surface on the Reactivity: Influence on Ethylene, Propylene, and 1,3-Butadiene Homopolymerization
Inorganic Chemistry, (55): 10024-10033. 2016. 10.1021/acs.inorgchem.6b01238

- Delarami, H. S.; Ebrahimi, A.
Theoretical investigation of the backbone center dot center dot center dot pi and pi center dot center dot center dot pi stacking interactions in substituted-benzene//3-methyl-2'-deoxyadenosine: a perspective to the DNA repair
Molecular Physics, (114): 774-783. 2016. 10.1080/00268976.2015.1118569
- Demir, S.; Sarioglu, A. O.; Guler, S.; Dege, N.; Sonmez, M.
Synthesis, crystal structure analysis, spectral IR, NMR UV-Vis investigations, NBO and NLO of 2-benzoyl-N-(4-chlorophenyl)-3-oxo-3-phenylpropanamide with use of X-ray diffractions studies along with DFT calculations
Journal of Molecular Structure, (1118): 316-324. 2016. 10.1016/j.molstruc.2016.04.042
- Demir, S.; Tinmaz, F.; Dege, N.; Ilhan, I. O.
Vibrational spectroscopic studies, NMR, HOMO-LUMO, NLO and NBO analysis of 1-(2-nitrobenzoyl)-3,5-diphenyl-4,5-dihydro-1H-pyrazole with use X-ray diffractions and DFT calculations
Journal of Molecular Structure, (1108): 637-648. 2016. 10.1016/j.molstruc.2015.12.057
- Demissie, T. B.; Ashebir, G. Y.
DIVERSION OF THE MELANIN SYNTHETIC PATHWAY BY DOPAMINE PRODUCT SCAVENGERS: A QUANTUM CHEMICAL MODELING OF THE REACTION MECHANISMS
Bulletin of the Chemical Society of Ethiopia, (30): 437-448. 2016. 10.4314/bcse.v30i3.12
- Demissie, T. B.; Hansen, J. H.
Mechanism and Site Selectivity in Visible-Light Photocatalyzed C-H Functionalization: Insights from DFT Calculations
Journal of Organic Chemistry, (81): 7110-7120. 2016. 10.1021/acs.joc.6b00977
- Demoin, D. W.; Dame, A. N.; Minard, W. D.; Gallazzi, F.; Seickman, G. L.; Rold, T. L.; Bernskoetter, N.; Fassbender, M. E.; Hoffman, T. J.; Deakyne, C. A.; Jurisson, S. S.
*Monooxorhenium(V) complexes with 222-N2S2 MAMA ligands for bifunctional chelator agents: Syntheses and preliminary *in vivo* evaluation*
Nuclear Medicine and Biology, (43): 802-811. 2016. 10.1016/j.nucmedbio.2016.08.017
- Denegri, B.; Matic, M.; Kronja, O.
The Role of Negative Hyperconjugation in Decomposition of Bicarbonate and Organic Carbonate Anions
Chemistryselect, (1): 5250-5259. 2016. 10.1002/slct.201601357
- Deng, X. J.; Kong, X. Y.; Xu, X. L.; Xu, H. G.; Zheng, W. J.
Photoelectron Spectroscopy and Density Functional Calculations of TiGen-(n=7-12) Clusters
Chinese Journal of Chemical Physics, (29): 123-128. 2016. 10.1063/1674-0068/29/cjcp1511232
- Dengel, H.; Lichtenberg, C.
Cationic Bismuth Amides: Accessibility, Structure, and Reactivity
Chemistry-a European Journal, (22): 18465-18475. 2016. 10.1002/chem.201604117
- Derikvand, Z.; Zabardasti, A.; Azadbakht, A.
Intermolecular complexes of nido-C₂B₃H₇ with HF and LiH molecules: the theoretical studies, bonding properties and natural bond orbital (NBO) analysis
Structural Chemistry, (27): 477-485. 2016. 10.1007/s11224-015-0576-x
- Devi, P. K.; Venkatachalam, K.
Structural, optical, mechanical and density functional theory studies of 1H-pyrazol-2-i um hydrogen oxalate crystal
Materials Chemistry and Physics, (183): 210-219. 2016. 10.1016/j.matchemphys.2016.08.020
- Devi, P. K.; Venkatachalam, K.; Poonkothai, M.
Spectroscopic, optical, thermal, antimicrobial and density functional theory studies of 4-aminopyridinium 4-hydroxy benzoate hydrate crystal
Journal of Molecular Structure, (1119): 462-471. 2016. 10.1016/j.molstruc.2016.05.001
- Devillard, M.; Lamsfus, C. A.; Vreeken, V.; Maron, L.; van der Vlugt, J. I.
Versatile coordination of a reactive P,N-ligand toward boron, aluminum and gallium and interconversion reactivity

Dalton Transactions, (45): 10989-10998. 2016. 10.1039/c6dt02087a

Dewberry, C. T.; Cornelius, R. D.; Mackenzie, R. B.; Smith, C. J.; Dvorak, M. A.; Leopold, K. R.

Microwave spectrum and structure of the 3,5-difluoropyridine...CO₂ van der Waals complex

Journal of Molecular Spectroscopy, (328): 67-72. 2016. 10.1016/j.jms.2016.08.016

Dey, D.; Sarangi, M. K.; Ray, A.; Bhattacharyya, D.; Maity, D. K.

Excited state hydrogen bonding fluorescent probe: Role of structure and environment

Journal of Luminescence, (173): 105-112. 2016. 10.1016/j.jlumin.2015.12.011

Dhara, A. K.; Singh, U. P.; Ghosh, K.

Radical pathways and O-2 participation in benzyl alcohol oxidation, and catechol and o-amino-phenol oxidase activity

studies with novel zinc complexes: an experimental and theoretical investigation

Inorganic Chemistry Frontiers, (3): 1543-1558. 2016. 10.1039/c6qi00356g

Di Pietro, P.; Kerridge, A.

U-O-yl Stretching Vibrations as a Quantitative Measure of the Equatorial Bond Covalency in Uranyl Complexes: A

Quantum-Chemical Investigation

Inorganic Chemistry, (55): 573-583. 2016. 10.1021/acs.inorgchem.5b01219

Die, D.; Zheng, B. X.; Zhao, L. Q.; Zhu, Q. W.; Zhao, Z. Q.

Insights into the structural, electronic and magnetic properties of V-doped copper clusters: comparison with pure copper clusters

Scientific Reports, (6) 2016. 10.1038/srep31978

Dimic, D.; Petkovic, M.

Control of a Photoswitching Chelator by Metal Ions: DFT, NBO, and QTAIM Analysis

International Journal of Quantum Chemistry, (116): 27-34. 2016. 10.1002/qua.25018

Ding, X.; Gou, R. J.; Ren, F. D.; Liu, F.; Zhang, S. H.; Gao, H. F.

Molecular Dynamics Simulation and Density Functional Theory Insight into the Cocrystal Explosive of Hexaaazaisowurtzitane/Nitroguanidine

International Journal of Quantum Chemistry, (116): 88-96. 2016. 10.1002/qua.25027

Dinparast, L.; Valizadeh, H.; Vessally, E.; Bahadori, M. B.

Synthesis, characterization and DFT studies of diethyl 4-hydroxy-6-nitro-4H-chromene-2,3-dicarboxylate

Journal of Molecular Structure, (1105): 118-127. 2016. 10.1016/j.molstruc.2015.10.044

Ditchfield, R.; Spencer, T. A.

Carbocation-pi interaction: evaluation of the stabilization by phenylalanine of a biochemical carbocation intermediate

Organic & Biomolecular Chemistry, (14): 9543-9548. 2016. 10.1039/c6ob01761d

Dodziuk, H.; Ruud, K.; Korona, T.; Demissie, T. B.

Chiral recognition by fullerenes: CHFCIBr enantiomers in the C-82 cage

Physical Chemistry Chemical Physics, (18): 26057-26068. 2016. 10.1039/c6cp05030a

Dolati, F.; Tayyari, S. F.; Vakili, M.; Ebrahimi, A.

Vibrational spectra of alpha-bromo and alpha-chloro derivatives of tris(acetylacetonato)chromium(III)

Journal of Molecular Structure, (1103): 1-8. 2016. 10.1016/j.molstruc.2015.09.012

Dolati, F.; Tayyari, S. F.; Vakili, M.; Wang, Y. A.

Proton transfer in acetylacetone and its alpha-halo derivatives

Physical Chemistry Chemical Physics, (18): 344-350. 2016. 10.1039/c5cp03845f

Domingo, L. R.

Molecular Electron Density Theory: A Modern View of Reactivity in Organic Chemistry

Molecules, (21) 2016. 10.3390/molecules21101319

- Domingo, L. R.; Emamian, S.; Salami, M.; Rios-Gutierrez, M.
Understanding the molecular mechanism of the 3+2 cycloaddition reaction of benzonitrile oxide toward electron-rich N-vinylpyrrole: a DFT study
Journal of Physical Organic Chemistry, (29): 368-376. 2016. 10.1002/poc.3544
- Domingo, L. R.; Rios-Gutierrez, M.; Chamorro, E.; Perez, P.
Electrophilic activation of CO₂ in cycloaddition reactions towards a nucleophilic carbenoid intermediate: new defying insights from the Molecular Electron Density Theory
Theoretical Chemistry Accounts, (136) 2016. 10.1007/s00214-016-2022-6
- Domingo, L. R.; Rios-Gutierrez, M.; Duque-Norena, M.; Chamorro, E.; Perez, P.
Understanding the carbenoid-type reactivity of nitrile ylides in 3+2 cycloaddition reactions towards electron-deficient ethylenes: a molecular electron density theory study
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1909-6
- Domingo, L. R.; Rios-Gutierrez, M.; Emamian, S.
Understanding the stereoselectivity in Bronsted acid catalysed Povarov reactions generating cis/trans CF₃-substituted tetrahydroquinolines: a DFT study
RSC Advances, (6): 17064-17073. 2016. 10.1039/c5ra27650k
- Domingo, L. R.; Rios-Gutierrez, M.; Perez, P.
An MEDT study of the carbenoid-type 3+2 cycloaddition reactions of nitrile ylides with electron-deficient chiral oxazolidinones
Organic & Biomolecular Chemistry, (14): 10427-10436. 2016. 10.1039/c6ob01989g
- Domingo, L. R.; Rios-Gutierrez, M.; Perez, P.
A new model for C-C bond formation processes derived from the Molecular Electron Density Theory in the study of the mechanism of 3+2 cycloaddition reactions of carbenoid nitrile ylides with electron-deficient ethylenes
Tetrahedron, (72): 1524-1532. 2016. 10.1016/j.tet.2016.01.061
- Domingo, L. R.; Rios-Gutierrez, M.; Perez, P.; Chamorro, E.
Understanding the 2n+2n reaction mechanism between a carbenoid intermediate and CO₂
Molecular Physics, (114): 1374-1391. 2016. 10.1080/00268976.2016.1142127
- Dong, C. C.; Li, D. Z.; Zheng, X. D.
Structure and Chemical Bonding of the B₃S (n) (0/-) (n=2-4) Boron Sulfide Clusters: A Density Functional Theory Investigation
Journal of Cluster Science, (27): 1591-1600. 2016. 10.1007/s10876-016-1026-7
- Dong, K.; Zhang, S. J.; Wang, J. J.
Understanding the hydrogen bonds in ionic liquids and their roles in properties and reactions
Chemical Communications, (52): 6744-6764. 2016. 10.1039/c5cc10120d
- Dong, X. Y.; Li, X.; Li, B.; Zhu, Y. Y.; Zang, S. Q.; Tang, M. S.
Water sandwiched by a pair of aromatic rings in a proton-conducting metal-organic framework
Dalton Transactions, (45): 18142-18146. 2016. 10.1039/c6dt03632e
- Dong, Z. W.; Reinhold, C. R. W.; Schmidtmann, M.; Muller, T.
A Germylene Stabilized by Homoconjugation
Angewandte Chemie-International Edition, (55): 15899-15904. 2016. 10.1002/anie.201609576
- Dore, E. M.; Lyon, J. T.
The Structures of Silicon Clusters Doped with Two Gold Atoms, Si (n) Au-2 (n=1-10)
Journal of Cluster Science, (27): 1365-1381. 2016. 10.1007/s10876-016-1006-y
- Dorris, R. E.; Trendell, W. C.; Peebles, R. A.; Peebles, S. A.
Rotational Spectrum, Structure, and Interaction Energy of the Trifluoroethylene center dot center dot center dot Carbon Dioxide Complex

Journal of Physical Chemistry A, (120): 7865-7872. 2016. 10.1021/acs.jpca.6b08286

Dostanic, J.; Loncarevic, D.; Zlatar, M.; Vlahovic, F.; Jovanovic, D. M.

Quantitative structure-activity relationship analysis of substituted arylazo pyridone dyes in photocatalytic system: Experimental and theoretical study

Journal of Hazardous Materials, (316): 26-33. 2016. 10.1016/j.jhazmat.2016.05.015

Dragancea, D.; Talmaci, N.; Shova, S.; Novitchi, G.; Darvasiova, D.; Rapta, P.; Breza, M.; Galanski, M.; Kozisek, J.; Martins, N. M. R.; Martins, L.; Pombeiro, A. J. L.; Arion, V. B.

Vanadium(V) Complexes with Substituted 1,5-bis(2-hydroxybenzaldehyde)carbohydrazones and Their Use As Catalyst Precursors in Oxidation of Cyclohexane

Inorganic Chemistry, (55): 9187-9203. 2016. 10.1021/acs.inorgchem.6b01011

Driver, R. W.; Claridge, T. D. W.; Scheiner, S.; Smith, M. D.

Torsional and Electronic Factors Control the C-H center dot center dot center dot O Interaction
Chemistry-a European Journal, (22): 16513-16521. 2016. 10.1002/chem.201602905

Drover, M. W.; Bowes, E. G.; Schafer, L. L.; Love, J. A.; Weller, A. S.

*Phosphoramidate-Supported Cp*Ir-III Aminoborane H2B=NR2 Complexes: Synthesis, Structure, and Solution Dynamics*
Chemistry-a European Journal, (22): 6793-6797. 2016. 10.1002/chem.201600951

Du, J. G.; Sun, X. Y.; Jiang, G.

Exploring the Interaction Natures in Plutonyl (VI) Complexes with Topological Analyses of Electron Density
International Journal of Molecular Sciences, (17) 2016. 10.3390/ijms17040414

Du, R. B.; Yu, D. H.; An, H. Y.; Zhang, S. H.; Lu, R. J.; Zhao, G.; Xiao, J. C.

alpha,beta-Substituent effect of dialkylphosphinic acids on lanthanide extraction
RSC Advances, (6): 56004-56008. 2016. 10.1039/c6ra10214j

Duan, X. F. F.; Burggraf, L. W.

The closo-Si12C12 molecule from cluster to crystal: A theoretical prediction
Journal of Chemical Physics, (144) 2016. 10.1063/1.4943957

Duan, Y. Q.; Liu, Y. X.; Bi, S. W.; Ling, B. P.; Jiang, Y. Y.; Liu, P.

Theoretical Study of Gold-Catalyzed Cyclization of 2-Alkynyl-N-propargylanilines and Rationalization of Kinetic Experimental Phenomena
Journal of Organic Chemistry, (81): 9381-9388. 2016. 10.1021/acs.joc.6b02092

Duanmu, K.; Roberto-Neto, O.; Machado, F. B. C.; Hansen, J. A.; Shen, J.; Piecuch, P.; Truhlar, D. G.

Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg-n(0,+/- 1), n=1-7
Journal of Physical Chemistry C, (120): 13275-13286. 2016. 10.1021/acs.jpcc.6b03080

Duarte, D. J. R.; Miranda, M. S.; da Silva, J.; Liebman, J. F.

A theoretical study of the strong interactions between carbon dioxide and OH+ and NH2 (+) products resulting from protonation of 1,2-dioxirane-3-one and 1,2-oxaziridine-3-one, respectively
Structural Chemistry, (27): 1743-1751. 2016. 10.1007/s11224-016-0794-x

Ducati, L. C.; Marchenko, A.; Autschbach, J.

NMR J-Coupling Constants of Ti-Pt Bonded Metal Complexes in Aqueous Solution: Ab Initio Molecular Dynamics and Localized Orbital Analysis
Inorganic Chemistry, (55): 12011-12023. 2016. 10.1021/acs.inorgchem.6b02180

Dudev, T.; Grauffel, C.; Lim, C.

Influence of the Selectivity Filter Properties on Proton Selectivity in the Influenza A M2 Channel
Journal of the American Chemical Society, (138): 13038-13047. 2016. 10.1021/jacs.6b08041

Dudev, T.; Mazmanian, K.; Lim, C.

Factors controlling the selectivity for Na+ over Mg2+ in sodium transporters and enzymes

Physical Chemistry Chemical Physics, (18): 16986-16997. 2016. 10.1039/c6cp01937d

Duignan, T. J.; Autschbach, J.

Impact of the Kohn-Sham Delocalization Error on the 4f Shell Localization and Population in Lanthanide Complexes
Journal of Chemical Theory and Computation, (12): 3109-3121. 2016. 10.1021/acs.jctc.6b00238

Dulski, M.; Cecotka, A.; Tripathy, S. N.; Sakalouski, A.; Wolnica, K.; Tarnacka, M.; Wrzalik, R.; Kaminski, K.; Paluch, M.
Experimental (FTIR, BDS) and theoretical analysis of mutarotation kinetics of D-fructose mixed with different alcohols in the supercooled region
RSC Advances, (6): S7634-S7646. 2016. 10.1039/c6ra13266a

Dumas, T.; Guillaumont, D.; Filliaux, C.; Scheinost, A.; Moisy, P.; Petit, S.; Shuh, D. K.; Tyliszczak, T.; Den Auwer, C.
The nature of chemical bonding in actinide and lanthanide ferrocyanides determined by X-ray absorption spectroscopy and density functional theory
Physical Chemistry Chemical Physics, (18): 2887-2895. 2016. 10.1039/c5cp05820a

Duran, R.; Vohringer-Martinez, E.; Toro-Labbe, A.; Herrera, B.
Reaction electronic flux and its role in DNA intramolecular proton transfers
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2989-x

Durandin, N. A.; Tsvetkov, V. B.; Bykov, E. E.; Kaluzhny, D. N.; Lavrenov, S. N.; Tevyashova, A. N.; Preobrazhenskaya, M. N.
Quantitative parameters of complexes of tris(1-alkylindol-3-yl) methylum salts with serum albumin: Relevance for the design of drug candidates
Journal of Photochemistry and Photobiology B-Biology, (162): 570-576. 2016. 10.1016/j.jphotobiol.2016.07.017

Dureckova, H.; Woo, T. K.; Alavi, S.
Molecular simulations and density functional theory calculations of bromine in clathrate hydrate phases
Journal of Chemical Physics, (144) 2016. 10.1063/1.4940321

Durgun, M.; Ceylan, U.; Yalcin, S. P.; Turkmen, H.; Ozdemir, N.; Koyuncu, I.
Synthesis, molecular structure, spectroscopic characterization, NBO, NLO and NPA analysis and in vitro cytotoxicity study of 3-chloro-N-(4-sulfamoylphenethyl)propanamide with experimental and computational study
Journal of Molecular Structure, (1114): 95-107. 2016. 10.1016/j.molstruc.2016.02.062

Dutta, D.; Tummanapelli, A. K.
Spectroscopic and computational investigations on the origin of charge transfer between included neutral guest molecules and a functionalized anionic layered host
Physical Chemistry Chemical Physics, (18): 22379-22389. 2016. 10.1039/c6cp03329f

Ehsani, A.
Inhibitory effect of new oxazol derivative on corrosion of stainless steel in acidic medium: An electrochemical investigation
Indian Journal of Chemical Technology, (23): 289-295. 2016.

Ehsani, A.; Shiri, H. M.
Electrochemical investigation of inhibitory of new synthesized 3-(4-iodophenyl)-2-imino-2,3-dihydrobenzo d oxazol-5-yl 4-methylbenzenesulfonate on corrosion of al in acidic medium
Protection of Metals and Physical Chemistry of Surfaces, (52): 348-355. 2016. 10.1134/s2070205116020088

Ehsani, A.; Shiri, H. M.; Mahjani, M. G.; Moshrefi, R.; Hadi, M.; Soltanpour, N.
Theoretical, common electrochemical and electrochemical noise investigation of inhibitory effect of new organic compound nanoparticles in the corrosion of stainless steel in acidic solution
Transactions of the Indian Institute of Metals, (69): 1519-1527. 2016. 10.1007/s12666-015-0724-4

El Bakouri, O.; Duran, M.; Poater, J.; Feixas, F.; Sola, M.
Octahedral aromaticity in (2S+1)A(1g) X-6(q) clusters (X = Li-C and Be-Si, S=0-3, and q =-2 to +4)
Physical Chemistry Chemical Physics, (18): 11700-11706. 2016. 10.1039/c5cp07011b

- El Mahdy, A. M.
Density functional investigation of CO and NO adsorption on TM-decorated C-60 fullerene
Applied Surface Science, (383): 353-366. 2016. 10.1016/j.apsusc.2016.04.037
- El-Azab, A. S.; Jalaja, K.; Abdel-Aziz, A. A. M.; Al-Obaid, A. M.; Mary, Y. S.; Panicker, C. Y.; Van Alsenoy, C.
Spectroscopic analysis (FT-IR, FT-Raman and NMR) and molecular docking study of ethyl 2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)-acetate
Journal of Molecular Structure, (1119): 451-461. 2016. 10.1016/j.molstruc.2016.05.004
- El-Azab, A. S.; Mary, Y. S.; Panicker, C. Y.; Abdel-Aziz, A. A. M.; Al-Suwaidan, I. A.; Van Alsenoy, C.
FT-IR, FT-Raman and molecular docking study of ethyl 4-(2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)acetamido)benzoat e
Journal of Molecular Structure, (1111): 9-18. 2016. 10.1016/j.molstruc.2016.01.041
- El-Azab, A. S.; Mary, Y. S.; Panicker, C. Y.; Abdel-Aziz, A. A. M.; El-Sherbeny, M. A.; Van Alsenoy, C.
DFT and experimental (FT-IR and FT-Raman) investigation of vibrational spectroscopy and molecular docking studies of 2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)-N-(3,4,5-trimethoxy phenyl) acetamide
Journal of Molecular Structure, (1113): 133-145. 2016. 10.1016/j.molstruc.2016.02.038
- El-Daly, S. A.; Alamry, K. A.
Spectroscopic Investigation and Photophysics of a D-pi-A-pi-D Type Styryl Pyrazine Derivative
Journal of Fluorescence, (26): 163-176. 2016. 10.1007/s10895-015-1698-7
- El-Faham, A.; Soliman, S. M.; Ghabbour, H. A.; Elnakady, Y. A.; Mohaya, T. A.; Siddiqui, M. R. H.; Albericio, F.
Ultrasonic promoted synthesis of novel s-triazine-Schiff base derivatives; molecular structure, spectroscopic studies and their preliminary anti-proliferative activities
Journal of Molecular Structure, (1125): 121-135. 2016. 10.1016/j.molstruc.2016.06.061
- El-Faham, A.; Soliman, S. M.; Osman, S. M.; Ghabbour, H. A.; Siddiqui, M. R. H.; Fun, H. K.; Albericio, F.
One pot synthesis, molecular structure and spectroscopic studies (X-ray, IR, NMR, UV-Vis) of novel 2-(4,6-dimethoxy-1,3,5-triazin-2-yl) amino acid ester derivatives
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (159): 184-198. 2016.
10.1016/j.saa.2016.01.051
- Elleuch, N.; Abid, Y.; Feki, H.
Spectroscopic and theoretical study of the charge transfer interaction effect on the vibrational modes and nonlinear optical properties in L-asparaginium nitrate crystal
Journal of Molecular Structure, (1120): 79-85. 2016. 10.1016/j.molstruc.2016.05.016
- Elnajjar, F. O.; Binder, J. F.; Kosnik, S. C.; Macdonald, C. L. B.
1,2,4-Triazol-5-ylidenes versus Imidazol-2-ylidenes for the Stabilization of Phosphorus(I) Cations
Zeitschrift fur Anorganische und Allgemeine Chemie, (642): 1251-1258. 2016. 10.1002/zaac.201600270
- Elroby, S. A.
Tautomerization, acidity, basicity, and stability of cyanoform: a computational study
Chemistry Central Journal, (10) 2016. 10.1186/s13065-016-0166-z
- Emamian, S.
How the mechanism of a 3+2 cycloaddition reaction involving a stabilized N-lithiated azomethine ylide toward a pi-deficient alkene is changed to stepwise by solvent polarity? What is the origin of its regio- and endo stereospecificity? A DFT study using NBO, QTAIM, and NCI analyses
RSC Advances, (6): 75299-75314. 2016. 10.1039/c6ra13913b
- Enescu, M.; Nagy, K. L.; Manceau, A.
Nucleation of mercury sulfide by dealkylation
Scientific Reports, (6) 2016. 10.1038/srep39359
- Erickson, J. D.; Mednikov, E. G.; Ivanov, S. A.; Dahl, L. F.

Isolation and Structural Characterization of a Mackay 55-Metal-Atom Two-Shell Icosahedron of Pseudo-I-h Symmetry, Pd₅₅L₁₂(mu(3)-CO)20 (L = PR₃, R = Isopropyl): Comparative Analysis with Interior Two-Shell Icosahedral Geometries in Capped Three-Shell Pd-145, Pt-Centered Four-Shell Pd-Pt M-165, and Four-Shell Au-133 Nanoclusters
Journal of the American Chemical Society, (138): 1502-1505. 2016. 10.1021/jacs.5b13076

Escobedo-Gonzalez, R.; Mendez-Albores, A.; Villarreal-Barajas, T.; Aceves-Hernandez, J. M.; Miranda-Ruvalcaba, R.; Nicolas-Vazquez, I.
A Theoretical Study of 8-Chloro-9-Hydroxy-Aflatoxin B-1, the Conversion Product of Aflatoxin B-1 by Neutral Electrolyzed Water
Toxins, (8) 2016. 10.3390/toxins8070225

Eskandari, K.
Nature of beryllium bonds in view of interacting quantum atoms and natural energy decomposition analysis
Computational and Theoretical Chemistry, (1090): 74-79. 2016. 10.1016/j.comptc.2016.06.005

Esme, A.; Sagdinc, S. G.
Theoretical Studies of Molecular Structures, Infrared Spectra, NBO and NLO Properties of Some Novel 5-arylazo-6-hydroxy-4-phenyl-3-cyano-2-pyridone Dyes
Acta Physica Polonica A, (130): 1273-1287. 2016. 10.12693/APhysPolA.130.1273

Espinosa, S.; Lezama, J.; Mora, J. R.; Cordova, T.; Chuchani, G.
Theoretical calculations on the mechanism of the elimination kinetics of allyl cyclohexyl-, -amine, -sulfide, -ether, and allyl ethyl ether in the gas phase
Computational and Theoretical Chemistry, (1090): 6-16. 2016. 10.1016/j.comptc.2016.05.010

Esrafilii, M. D.; Akhgarpour, H.
An ab initio study on competition between pnicogen and chalcogen bond interactions in binary XHS:PH₂X complexes (X = F, Cl, CCH, COH, CH₃, OH, OCH₃ and NH₂)
Molecular Physics, (114): 1847-1855. 2016. 10.1080/00268976.2016.1158421

Esrafilii, M. D.; Amiri, Z.; Shankal, F.
Strong cooperative effects between pi-hole and dihydrogen bonds interactions: a computational study
Molecular Physics, (114): 2315-2324. 2016. 10.1080/00268976.2016.1203037

Esrafilii, M. D.; Asadollahi, S.
Cationic P center dot center dot center dot N interaction in XH₃P+center dot center dot center dot NCY complexes (X = H, F, CN, NH₂, OH; Y = H, Li, F, Cl) and its cooperativity with hydrogen/lithium/halogen bond
Journal of Molecular Graphics & Modelling, (64): 131-138. 2016. 10.1016/j.jmgm.2016.01.011

Esrafilii, M. D.; Asadollahi, S.; Shahamat, Y. D.
Competition between chalcogen bond and halogen bond interactions in YOX₄:NH₃ (Y = S, Se; X = F, Cl, Br) complexes: An ab initio investigation
Structural Chemistry, (27): 1439-1447. 2016. 10.1007/s11224-016-0763-4

Esrafilii, M. D.; Asadollahi, S.; Shahamat, Y. D.
The mutual influence of Y center dot center dot center dot N and H center dot center dot center dot H interactions in XHY center dot center dot center dot NCH center dot center dot center dot HM complexes (X = F, Cl, Br; Y = S, Se; M = Li, Na, BeH, MgH): tuning of the chalcogen bond by dihydrogen bond interaction
Canadian Journal of Chemistry, (94): 567-573. 2016. 10.1139/cjc-2016-0052

Esrafilii, M. D.; Asadollahi, S.; Vakili, M.
Investigation of substituent effects in aerogen-bonding interaction between ZO(3) (Z=Kr, Xe) and nitrogen bases
International Journal of Quantum Chemistry, (116): 1254-1260. 2016. 10.1002/qua.25168

Esrafilii, M. D.; Kiani, H.; Mohammadian-Sabet, F.
Tuning of carbon bonds by substituent effects: an ab initio study
Molecular Physics, (114): 3658-3668. 2016. 10.1080/00268976.2016.1255800

- Esrafilii, M. D.; Mohammadian-Sabet, F.
An ab initio study on cationic chalcogen bond interactions between F3-nHnS+ (n=0-2) and nitrogen bases
Chemical Physics Letters, (645): 32-37. 2016. 10.1016/j.cplett.2015.12.027
- Esrafilii, M. D.; Mohammadian-Sabet, F.
Cooperativity of tetrel bonds tuned by substituent effects
Molecular Physics, (114): 1528-1538. 2016. 10.1080/00268976.2016.1139207
- Esrafilii, M. D.; Mohammadian-Sabet, F.
Exploring "aerogen-hydride" interactions between ZOF(2) (Z = Kr, Xe) and metal hydrides: An ab initio study
Chemical Physics Letters, (654): 23-28. 2016. 10.1016/j.cplett.2016.05.010
- Esrafilii, M. D.; Mohammadian-Sabet, F.
Homonuclear chalcogen-chalcogen bond interactions in complexes pairing YO3 and YHX molecules (Y=S, Se; X=H, Cl, Br, CCH, NC, OH, OCH3): Influence of substitution and cooperativity
International Journal of Quantum Chemistry, (116): 529-536. 2016. 10.1002/qua.25076
- Esrafilii, M. D.; Mohammadian-Sabet, F.
Substituent effects on geometry and bonding properties of asymmetric bifurcated pnicogen bonds: A theoretical study
Chemical Physics Letters, (650): 52-56. 2016. 10.1016/j.cplett.2016.02.060
- Esrafilii, M. D.; Mohammadian-Sabet, F.
Theoretical insights into nature of pi-hole interactions between triel centers (B and Al) and radical methyl as a potential electron donor: Do single-electron triel bonds exist?
Structural Chemistry, (27): 1157-1164. 2016. 10.1007/s11224-015-0739-9
- Esrafilii, M. D.; Mohammadian-Sabet, F.
Tuning tetrel bonds via cation-pi interactions: an ab initio study on concerted interaction in M+-C6H5XH3-NCY complexes (M= Li, Na, K; X = Si, Ge; Y = H, F, OH)
Molecular Physics, (114): 83-91. 2016. 10.1080/00268976.2015.1086498
- Esrafilii, M. D.; Mohammadian-Sabet, F.; Nematollahi, P.
Oxidation of CO by N2O over Al- and Ti-doped graphene: a comparative study
RSC Advances, (6): 64832-64840. 2016. 10.1039/c6ra04326g
- Esrafilii, M. D.; Mohammadian-Sabet, F.; Solimannejad, M.
Single-electron aerogen bonds: Do they exist?
Chemical Physics Letters, (659): 196-202. 2016. 10.1016/j.cplett.2016.07.025
- Esrafilii, M. D.; Mohammadian-Sabet, F.; Vessally, E.
An ab initio study on the nature of sigma-hole interactions in pnicogen-bonded complexes with carbene as an electron donor
Molecular Physics, (114): 2115-2122. 2016. 10.1080/00268976.2016.1185547
- Esrafilii, M. D.; Nematollahi, P.; Nurazar, R.
A density functional theory study on adsorption and decomposition of acetic acid over silicon carbide nanotubes
Synthetic Metals, (215): 164-169. 2016. 10.1016/j.synthmet.2016.02.019
- Esrafilii, M. D.; Nematollahi, P.; Nurazar, R.
Pd-embedded graphene: An efficient and highly active catalyst for oxidation of CO
Superlattices and Microstructures, (92): 60-67. 2016. 10.1016/j.spmi.2016.02.006
- Esrafilii, M. D.; Saeidi, N.; Nematollahi, P.
A DFT study on SO3 capture and activation over Si- or Al-doped graphene
Chemical Physics Letters, (658): 146-151. 2016. 10.1016/j.cplett.2016.06.045
- Esrafilii, M. D.; Saeidi, N.; Nematollahi, P.
The healing of B- or N-vacancy defective BNNTs by using CO molecule: a DFT study

New Journal of Chemistry, (40): 8024-8031. 2016. 10.1039/c6nj00921b

Esrafil, M. D.; Saeidi, N.; Nematollahi, P.

Si-doped graphene: A promising metal-free catalyst for oxidation of SO₂
Chemical Physics Letters, (649): 37-43. 2016. 10.1016/j.cplett.2016.02.028

Esrafil, M. D.; Vessally, E.

The strengthening effect of a hydrogen or lithium bond on the Z center dot center dot center dot N aerogen bond (Z = Ar, Kr and Xe): a comparative study
Molecular Physics, (114): 3265-3276. 2016. 10.1080/00268976.2016.1227097

Esrafil, M. D.; Vessally, E.

A theoretical evidence for cooperative enhancement in aerogen-bonding interactions: Open-chain clusters of KrOF₂ and XeOF₂
Chemical Physics Letters, (662): 80-85. 2016. 10.1016/j.cplett.2016.09.037

Esrafil, M. D.; Vessally, E.; Solimannejad, M.

Symmetric bifurcated halogen bonds: substituent and cooperative effects
Molecular Physics, (114): 3610-3619. 2016. 10.1080/00268976.2016.1253882

Esselman, B. J.; Hill, N. J.

Integration of Computational Chemistry into the Undergraduate Organic Chemistry Laboratory Curriculum
Journal of Chemical Education, (93): 932-936. 2016. 10.1021/acs.jchemed.5b00815

Esterhuysen, C.; Ford, T. A.

Ab initio studies of the structures and vibrational spectra of the hydrogen halide and lithium halide homo- and heterodimers and some mixed hydrogen halide/lithium halide heterodimers
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1949-y

Estevez-Hernandez, O.; Salomon, F. F.; Duque, J.; Rodriguez-Hernandez, J.; Gil, D. M.

Synthesis, structural and spectroscopic studies of 1-(2-FUROYL)-3-phenylthiourea: a theoretical and experimental approach
Journal of Sulfur Chemistry, (37): 555-579. 2016. 10.1080/17415993.2016.1209755

Etminan, N.; Yoosefian, M.; Raissi, H.; Hakimi, M.

Solvent effects on the stability and the electronic properties of histidine/Pd-doped single-walled carbon nanotube biosensor
Journal of Molecular Liquids, (214): 313-318. 2016. 10.1016/j.molliq.2015.12.009

Evecen, M.; Tanak, H.

Quantum chemical studies on the molecular structure, spectroscopic and electronic properties of (6-Methoxy-2-oxo-2H-chromen-4-yl)-methyl pyrrolidine-1-carbodithioate
Materials Science-Poland, (34): 886-904. 2016. 10.1515/msp-2016-0115

Evecen, M.; Tanak, H.; Tinmaz, F.; Dege, N.; Ilhan, I. O.

Experimental (XRD, IR and NMR) and theoretical investigations on 1-(2-nitrobenzoyl)3,5-bis(4-methoxyphenyl)-4,5-dihydro-1H-pyrazole
Journal of Molecular Structure, (1126): 117-126. 2016. 10.1016/j.molstruc.2016.01.069

Fakhraee, S.; Souri, M.

Double hydrogen bond interaction in 7-azaindole complexes with protic solvents
Journal of Molecular Graphics & Modelling, (70): 45-53. 2016. 10.1016/j.jmgm.2016.06.009

Fallahpour, F.; Gorgani, S. S.; Nouraliei, M.

Boron carbide nanoclusters as H-2 and N-2 gases nanosensors: theoretical investigation
Indian Journal of Physics, (90): 931-936. 2016. 10.1007/s12648-016-0834-9

Fallahpour, F.; Nouraliei, M.; Gorgani, S. S.

Theoretical evaluation of a double-functional heterogeneous nano-sensor
Applied Surface Science, (366): 545-551. 2016. 10.1016/j.apsusc.2016.01.051

Fan, Y. M.; Zhuo, Y. Q.; Zhu, Z. W.; Li, L. L.; Chen, Q.; Lou, Y.
Density functional theory study on Hg removal mechanisms of Cu-impregnated activated carbon prepared by simplified method
Korean Journal of Chemical Engineering, (33): 2869-2877. 2016. 10.1007/s11814-016-0153-z

Fang, T.; Gu, Y.; Huang, W.; Boons, G. J.
Mechanism of Glycosylation of Anomeric Sulfonium Ions
Journal of the American Chemical Society, (138): 3002-3011. 2016. 10.1021/jacs.5b08436

Fang, Z. T.; Thanthiriyawat, K. S.; Dixon, D. A.; Andrews, L.; Wang, X. F.
Properties of Cerium Hydroxides from Matrix Infrared Spectra and Electronic Structure Calculations
Inorganic Chemistry, (55): 1702-1714. 2016. 10.1021/acs.inorgchem.5b02619

Faponle, A. S.; Banse, F.; de Visser, S. P.
Arene activation by a nonheme iron(III)-hydroperoxo complex: pathways leading to phenol and ketone products
Journal of Biological Inorganic Chemistry, (21): 453-462. 2016. 10.1007/s00775-016-1354-y

Farrokhpour, H.; Karachi, S.; Chermahini, A. N.
Theoretical Modeling of the Chirality Discrimination of Enantiomers by Nanotubular Cyclic Peptides using Gas-Phase Photoelectron Spectroscopy: An ONIOM Spectroscopic Calculations
Journal of Physical Chemistry A, (120): 6780-6791. 2016. 10.1021/acs.jpca.6b07403

Farrokhzadeh, A.; Modarresi-Alam, A. R.; Akher, F. B.; Ebrahimi, A.
A theoretical study of pi-stacking interactions in C-substituted tetrazoles
Journal of Molecular Graphics & Modelling, (67): 85-93. 2016. 10.1016/j.jmgm.2016.05.005

Fasihizad, A.; Akbari, A.; Ahmadi, M.; Dusek, M.; Henriques, M. S.; Pojarova, M.
Copper(II) and molybdenum(VI) complexes of a tridentate ONN donor isothiosemicarbazole: Synthesis, characterization, X-ray, TGA and DFT
Polyhedron, (115): 297-305. 2016. 10.1016/j.poly.2016.05.018

Favero, L.; Crotti, P.; Di Bussolo, V.; Napolitano, E.
Regioselectivity and stereoselectivity of nucleophilic addition to glycal and imino-glycal vinyl epoxides and their carba analogs: a rationalization based on HSAB theory and MEP
Journal of Physical Organic Chemistry, (29): 234-243. 2016. 10.1002/poc.3525

Fedorova, I. V.; Safonova, L. P.
Influence of solvent environment using the CPCM model on the H-bond geometry in the complexes of phosphorus acids with DMSO
Structural Chemistry, (27): 1189-1198. 2016. 10.1007/s11224-016-0744-7

Feng, W. L.; Ren, C.; Wang, W. H.; Guo, C.; Sun, Q.; Li, P.
An identification of the C-C bonding spin adduct in the spin trapping of N-methyl benzohydroxamic acid radical by 5,5-dimethyl-1-pyrroline N-oxide
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1944-3

Feng, W. L.; Ren, C.; Wang, W. H.; Guo, C.; Sun, Q.; Li, P.
Theoretical studies on the spin trapping of the 2-chloro-5-hydroxy-1,4-benzoquinone radical by 5,5-dimethyl-1-pyrroline N-oxide (DMPO): the identification of the C-O bonding spin adduct
RSC Advances, (6): 48099-48108. 2016. 10.1039/c6ra07696c

Feng, X. L.; Li, N.; Lv, L. Q.; King, R. B.
Unsaturation in binuclear heterometallic carbonyls: the cyclopentadienyliron manganese carbonyl CpFeMn(CO)(n) system as a hybrid of the Cp₂Fe₂(CO)(n) and Mn-2(CO)(n) systems
New Journal of Chemistry, (40): 7482-7492. 2016. 10.1039/c5nj03459k

Ferao, A. E.; Afzal, F.; Aslam, S.; Muhammad, I. K.; Ejaz; Khan, I. U.; Fettouhi, M.; Isab, A. A.; Ahmad, S.
Synthesis, crystal structure and DFT calculations of bis(1,3-diazinane-2-thione- κ S)dicyanido disilver(I), {Ag(Diaz)(2)}{Ag(CN)(2)}
Polyhedron, (110): 299-304. 2016. 10.1016/j.poly.2015.10.028

Ferao, A. E.; Streubel, R.
Thiaphosphiranes and Their Complexes: Systematic Study on Ring Strain and Ring Cleavage Reactions
Inorganic Chemistry, (55): 9611-9619. 2016. 10.1021/acs.inorgchem.6b01322

Fernandez, I.; Cossio, F. P.
Interplay Between Aromaticity and Strain in Double Group Transfer Reactions to 1,2-Benzyne
Journal of Computational Chemistry, (37): 1265-1273. 2016. 10.1002/jcc.24317

Fernandez, L.; Perez-Pla, F. F.; Tunon, I.; Llopis, E.
DFT Study on the Interaction of Tris(benzene-1,2-dithiolato)molybdenum Complex with Water. A Hydrolysis Mechanism Involving a Feasible Seven-Coordinate Aquomolybdenum Intermediate
Journal of Physical Chemistry A, (120): 9636-9646. 2016. 10.1021/acs.jpca.6b10233

Feuerstein, W.; Hofener, S.; Klopper, W.; Lamparth, I.; Moszner, N.; Barner-Kowollik, C.; Unterreiner, A. N.
Photophysical Properties of Benzoylgermane and para-Substituted Derivatives: Substituent Effects on Electronic Transitions
Chemphyschem, (17): 3460-3469. 2016. 10.1002/cphc.201600712

Finkelmann, A. R.; Goller, A. H.; Schneider, G.
Robust molecular representations for modelling and design derived from atomic partial charges
Chemical Communications, (52): 681-684. 2016. 10.1039/c5cc07887c

Finney, B.; Fang, Z. T.; Francisco, J. S.; Dixon, D. A.
Energetic Properties and Electronic Structure of Si,N,S and Si,P,S Isomers
Journal of Physical Chemistry A, (120): 1691-1697. 2016. 10.1021/acs.jpca.6b00918

Finney, B.; Mitrushchenkov, A. O.; Francisco, J. S.; Peterson, K. A.
Ab initio ro-vibronic spectroscopy of the 2 Pi PCS radical and (1)Sigma+PCS- anion
Journal of Chemical Physics, (145) 2016. 10.1063/1.4971183

Firouzbakht, M.; Rijs, N. J.; Gonzalez-Navarrete, P.; Schlangen, M.; Kaupp, M.; Schwarz, H.
On the Activation of Methane and Carbon Dioxide by HTaO (+) and TaOH (+) in the Gas Phase: A Mechanistic Study
Chemistry-a European Journal, (22): 10581-10589. 2016. 10.1002/chem.201601339

Firouzbakht, M.; Schlangen, M.; Kaupp, M.; Schwarz, H.
Mechanistic aspects of CO₂ activation mediated by phenyl yttrium cation: A combined experimental/theoretical study
Journal of Catalysis, (343): 68-74. 2016. 10.1016/j.jcat.2015.09.012

Flores, M. E.; Shibue, T.; Sugimura, N.; Nishide, H.; Moreno-Villoslada, I.
Correlation between H-1 NMR chemical shifts of hydroxyl protons in n-hexanol/cyclohexane and molecular association properties investigated using density functional theory
Chemical Physics Letters, (644): 276-279. 2016. 10.1016/j.cplett.2015.12.025

Flores, R.; Castro, M.
Stability of one- and two-layers TM(Benzene)(m) (+/- 1), m <= 3; TM = Fe, Co, and Ni, complexes
Journal of Molecular Structure, (1125): 47-62. 2016. 10.1016/j.molstruc.2016.06.052

Flores, R.; Cortes, H. F.; Castro, M.
Probing the stability of the M-2(Benzene)(3) M = Fe, Co, and Ni structures upon electron attachment (deletion) and solvated iron clusters by benzene molecules: Fe-2(Benzene)(4)
Journal of Molecular Structure, (1103): 295-310. 2016. 10.1016/j.molstruc.2015.09.026

- Flores-Gallegos, N.
Informational energy as a measure of electron correlation
Chemical Physics Letters, (666): 62-67. 2016. 10.1016/j.cplett.2016.10.075
- Florez, E.; Acelas, N.; Ibarguen, C.; Mondal, S.; Cabellos, J. L.; Merino, G.; Restrepo, A.
Microsolvation of NO₃⁻: structural exploration and bonding analysis
RSC Advances, (6): 71913-71923. 2016. 10.1039/c6ra15059d
- Florez, E.; Merino, G.; Cabellos, J. L.; Ferraro, F.; Restrepo, A.; Hadad, C. Z.
Structure and bonding in WC_n (n=2-5) clusters
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1979-5
- Flyagina, I. S.; Hughes, K. J.; Mielczarek, D. C.; Ingham, D. B.; Pourkashanian, M.
Identifying the Catalytic Active Sites in Heteroatom-Doped Graphene for the Oxygen Reduction Reaction
Fuel Cells, (16): 568-576. 2016. 10.1002/fuce.201600019
- Forget, S. M.; Bushnell, E. A. C.; Boyd, R. J.; Jakeman, D. L.
The acidity of beta-phosphoglucomutase monofluoromethylenephosphonate ligands probed by NMR spectroscopy and quantum mechanical methods
Canadian Journal of Chemistry, (94): 902-908. 2016. 10.1139/cjc-2015-0477
- Fortino, M.; Marino, T.; Russo, N.; Sicilia, E.
A DFT investigation of a bulky biomimetic model catalyzing the 5'-outer ring deiodination of thyroxine
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3154-2
- Fortino, M.; Marino, T.; Russo, N.; Sicilia, E.
Mechanistic investigation of trimethylamine-N-oxide reduction catalysed by biomimetic molybdenum enzyme models
Physical Chemistry Chemical Physics, (18): 8428-8436. 2016. 10.1039/c5cp07278f
- Fouegue, A. D. T.; Ghogomu, J. N.; Mama, D. B.; Nkungli, N. K.; Younang, E.
Structural and Antioxidant Properties of Compounds Obtained from Fe²⁺ Chelation by Juglone and Two of Its Derivatives: DFT, QTAIM, and NBO Studies
Bioinorganic Chemistry and Applications, 2016. 10.1155/2016/8636409
- Francisco, E.; Casals-Sainz, J. L.; Rocha-Rinza, T.; Pendas, A. M.
Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1921-x
- Franco, J. M. V.; Schnakenburg, G.; Ferao, A. E.; Streubel, R.
Coordination chemistry of a low-coordinate non-metal element: the case of electrophilic terminal phosphinidene complexes
Dalton Transactions, (45): 13951-13956. 2016. 10.1039/c6dt02909d
- Fraser, R.; Van Rooyen, P. H.; Landman, M.
Conformational preferences of heteronuclear Fischer carbene complexes of cymantrene and cyclopentadienyl rhenium tricarbonyl
Journal of Coordination Chemistry, (69): 2972-2987. 2016. 10.1080/00958972.2016.1227071
- Fraser, R.; van Rooyen, P. H.; Landman, M.
Synthesis, structure and DFT study of cymantrenyl Fischer carbene complexes of group VI and VII transition metals
Journal of Molecular Structure, (1105): 178-185. 2016. 10.1016/j.molstruc.2015.10.051
- Fraser, R.; van Rooyen, P. H.; Landman, M.
Synthesis, structure and substitution pattern study of phosphine-substituted dimetallic Fischer carbene complexes of cymantrene
Polyhedron, (118): 133-142. 2016. 10.1016/j.poly.2016.08.010
- Fredin, L. A.; Warnmark, K.; Sundstrom, V.; Persson, P.

Molecular and Interfacial Calculations of Iron(II) Light Harvesters
Chemsuschem, (9): 667-675. 2016. 10.1002/cssc.201600062

Freitas, V. L. S.; Lima, A.; Sapei, E.; da Silva, M.
Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
Journal of Chemical Thermodynamics, (102): 287-292. 2016. 10.1016/j.jct.2016.07.015

Freitas, V. L. S.; Santos, C. P. F.; da Silva, M.; da Silva, M.
The effect of ketone groups on the energetic properties of phthalan derivatives
Journal of Chemical Thermodynamics, (96): 74-81. 2016. 10.1016/j.jct.2015.12.018

Frost, J. R.; Scully, C. C. G.; Yudin, A. K.
Oxadiazole grafts in peptide macrocycles
Nature Chemistry, (8): 1105-1111. 2016. 10.1038/nchem.2636

Fu, X. N.; Shang, Z. F.; Xu, X. F.
Rh(III)-Catalyzed Cascade Oxidative Annulation of Benzoylacetonitrile with Alkynes: Computational Study of Mechanism, Reactivity, and Regioselectivity
Journal of Organic Chemistry, (81): 8378-8385. 2016. 10.1021/acs.joc.6b01567

Fujita, Y.; Abe, M.; Shiota, Y.; Suzuki, T.; Yoshizawa, K.
Computational Study of Cyclobutane-1,3-diylidene Dicarbenes: Ground-State Spin Multiplicity and New Strategy toward the Synthesis of Bicyclo 1.1.0 but-1(3)-enes
Bulletin of the Chemical Society of Japan, (89): 770-778. 2016. 10.1246/bcsj.20160051

Funes-Ardoiz, I.; Sameera, W. M. C.; Romero, R. M.; Martinez, C.; Souto, J. A.; Sampedro, D.; Muniz, K.; Maseras, F.
DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes
Chemistry-a European Journal, (22): 7545-7553. 2016. 10.1002/chem.201600415

Furer, V. L.; Vandyukov, A. E.; Majoral, J. P.; Caminade, A. M.; Kovalenko, V. I.
Structure, IR and Raman spectra of phosphotrihydrazide studied by DFT
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (166): 19-24. 2016. 10.1016/j.saa.2016.04.047

Furer, V. L.; Vandyukov, A. E.; Padie, C.; Majoral, J. P.; Caminade, A. M.; Kovalenko, V. I.
FT-Raman, FT-IR spectroscopic and DFT studies of hexaphenoxycyclotriphosphazene
Journal of Molecular Structure, (1115): 124-135. 2016. 10.1016/j.molstruc.2016.02.097

Gadogbe, M.; Zhou, Y. D.; Zou, S. L.; Zhang, D. M.
Rigid Single Carbon-Carbon Bond That Does Not Rotate in Water
Journal of Physical Chemistry B, (120): 2418-2422. 2016. 10.1021/acs.jpcb.5b12166

Gadre, S. R.; Kumar, A.
Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules
Journal of Chemical Sciences, (128): 1519-1526. 2016. 10.1007/s12039-016-1160-7

Gai, X. Q.; Zhang, X. X.; Kang, J. J.; Xu, L.; Zhang, J. J.; Ni, J.
Effects of Different Amount of Crystalline Solvate Molecules on Solid Structures and Photophysical Properties of a Platinum(II) Moiety with 4,4'-Dibromo-2,2'-Bipyridine Ligand
Zeitschrift fur Anorganische und Allgemeine Chemie, (642): 597-602. 2016. 10.1002/zaac.201600073

Gajalakshmi; Tamilmani, V.
Unraveling the Role of Pi - Conjugation in Thiophene Oligomers for Optoelectronic Properties by DFT/TDDFT Approach
Brazilian Archives of Biology and Technology, (59) 2016. 10.1590/1678-4324-2016161015

Galabov, B.; Nalbantova, D.; Schleyer, P. V.; Schaefer, H. F.
Electrophilic Aromatic Substitution: New Insights into an Old Class of Reactions
Accounts of Chemical Research, (49): 1191-1199. 2016. 10.1021/acs.accounts.6b00120

- Galinato, M. G. I.; Fogle, R. S.; Stetz, A.; Galan, J. F.
Modulating the nitrite reductase activity of globins by varying the heme substituents: Utilizing myoglobin as a model system
Journal of Inorganic Biochemistry, (154): 7-20. 2016. 10.1016/j.jinorgbio.2015.10.010
- Gallardo-Fuentes, S.; Contreras, R.; Ormazabal-Toledo, R.
Origins of the ANRORC reactivity in nitroimidazole derivatives
RSC Advances, (6): 25215-25221. 2016. 10.1039/c6ra00199h
- Galvez, O.; Baeza-Romero, M. T.; Sanz, M.; Pacios, L. F.
A theoretical study on the reaction of ozone with aqueous iodide
Physical Chemistry Chemical Physics, (18): 7651-7660. 2016. 10.1039/c5cp06440f
- Gandhimathi, S.; Balakrishnan, C.; Venkataraman, R.; Neelakantan, M. A.
Crystal structure, solvatochromism and estimation of ground and excited state dipole moments of an allyl arm containing Schiff base: Experimental and theoretical calculations
Journal of Molecular Liquids, (219): 239-250. 2016. 10.1016/j.molliq.2016.02.097
- Gandomi, F.; Vakili, M.; Tayyari, S. F.
Vibrational spectra, normal coordinate analysis, and conformation of bis(alpha-cyanoacetylacetonato)Cu(II)
Journal of Molecular Structure, (1118): 68-74. 2016. 10.1016/j.molstruc.2016.03.101
- Ganesamoorthy, C.; Wolper, C.; Nizovtsev, A. S.; Schulz, S.
Synthesis and Structural Characterization of Magnesium-Substituted Polystibides (LMg)(4)Sb-8
Angewandte Chemie-International Edition, (55): 4204-4209. 2016. 10.1002/anie.201510504
- Ganesan, P.; Lakshmi pathi, S.
Influence of dopants Cu, Ga, In, Hg on the electronic structure of Cd_nSn (n=6, 15) clusters - a DFT study
RSC Advances, (6): 93056-93067. 2016. 10.1039/c6ra15049g
- Ganguly, A.; Paul, B. K.; Ghosh, S.; Guchhait, N.
Methanol-mediated excited-state double proton transfer in 1H-pyrrolo 3,2-h quinoline: Concerted or Sequential Mechanism?
Computational and Theoretical Chemistry, (1095): 65-70. 2016. 10.1016/j.comptc.2016.09.020
- Gani, T. Z. H.; Ioannidis, E. I.; Kulik, H. J.
Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation
Chemistry of Materials, (28): 6207-6218. 2016. 10.1021/acs.chemmater.6b02378
- Gani, T. Z. H.; Kulik, H. J.
Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT plus U
Journal of Chemical Theory and Computation, (12): 5931-5945. 2016. 10.1021/acs.jctc.6b00937
- Ganji, M. D.; Tajbakhsh, M.; Kariminasab, M.; Alinezhad, H.
Tuning the LUMO level of organic photovoltaic solar cells by conjugately fusing graphene flake: A DFT-B3LYP study
Physica E-Low-Dimensional Systems & Nanostructures, (81): 108-115. 2016. 10.1016/j.physe.2016.03.008
- Gao, S.; Lan, W. B.; Lin, Y. W.; Liao, L. F.; Nie, C. M.
Molecular Recognition of alpha,beta-Unsaturated Carbonyl Compounds and Chiral Guests by Uranyl-Salophen Receptors
Acta Physico-Chimica Sinica, (32): 683-690. 2016. 10.3866/pku.Whxb201512302
- Gao, Z. H.; Shi, Y. M.; Qiang, Z.; Wang, X.; Shang, S. Z.; Yang, Y.; Du, B. W.; Peng, H. P.; Ji, X.; Li, H. L.; Wang, F.; Xiao, W. L.
Plasiatine, an Unprecedented Indole-Phenylpropanoid Hybrid from Plantago asiatica as a Potent Activator of the Nonreceptor Protein Tyrosine Phosphatase Shp2
Scientific Reports, (6) 2016. 10.1038/srep24945
- Gapurenko, O. A.; Minyaev, R. M.; Minkin, V. I.; Lee, V. Y.; Sekiguchi, A.

Group 14 element cationic pentagonal-pyramidal complexes E-a eta(5)-E-5(b)(SiMe3)(5) (+) (E-a = Si-Pb, E-b = Si, Ge): A quantum-chemical study
Phosphorus Sulfur and Silicon and the Related Elements, (191): 609-612. 2016. 10.1080/10426507.2015.1128917

Garrett, B. R.; Polen, S. M.; Click, K. A.; He, M. F.; Huang, Z. J.; Hadad, C. M.; Wu, Y. Y.
Tunable Molecular MoS₂ Edge-Site Mimics for Catalytic Hydrogen Production
Inorganic Chemistry, (55): 3960-3966. 2016. 10.1021/acs.inorgchem.6b00206

Gasonoo, M.; Naredla, R. R.; Lill, S. O. N.; Klumpp, D. A.
Tetra- and Pentacationic Electrophiles and Their Chemistry
Journal of Organic Chemistry, (81): 11758-11765. 2016. 10.1021/acs.joc.6b02220

Gaudin, T.; Rotureau, P.; Pezron, I.; Fayet, G.
New QSPR Models to Predict the Critical Micelle Concentration of Sugar-Based Surfactants
Industrial & Engineering Chemistry Research, (55): 11716-11726. 2016. 10.1021/acs.iecr.6b02890

Gautam, S. K.; Maurya, H. K.; Pratap, R.; Kumar, B.; Kumar, A.; Tandon, V. K.; Ram, V. J.
Strategy to Construct Stair-Shaped Partially Reduced Naphtho 1,2-b pyrano 2,3-d oxepines and Dinaphtho 1,2-b,d oxepines
Journal of Heterocyclic Chemistry, (53): 2070-2078. 2016. 10.1002/jhet.2342

Gayen, B.; Banerji, A.; Dhara, K.
1,3-Dipolar cycloadditions of nonstabilized azomethine ylides to planar chalcones via regio- and stereoselective route: A three-component strategy
Synthetic Communications, (46): 293-308. 2016. 10.1080/00397911.2015.1135954

Ge, W. L.; Wang, X. C.; Zhang, L. Y.; Du, L.; Zhou, Y.; Wang, J.
Fully-occupied Keggin type polyoxometalate as solid base for catalyzing CO₂ cycloaddition and Knoevenagel condensation
Catalysis Science & Technology, (6): 460-467. 2016. 10.1039/c5cy01038a

Geethalakshmi, K. R.; Ng, T. Y.; Crespo-Otero, R.
Tunable optical properties of OH-functionalised graphene quantum dots
Journal of Materials Chemistry C, (4): 8429-8438. 2016. 10.1039/c6tc02785g

Gehrke, S.; Holloczki, O.
A molecular mechanical model for N-heterocyclic carbenes
Physical Chemistry Chemical Physics, (18): 22070-22080. 2016. 10.1039/c6cp02624a

Geng, B.; Xu, C. J.; Chen, Z. H.
Formation of the Si-B bond: insertion reactions of silylenes into B-X(X=F, Cl, Br, O, and N) bonds
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3006-0

Gentili, D.; Liscio, F.; Demitri, N.; Schafer, B.; Borgatti, F.; Torelli, P.; Gobaut, B.; Panaccione, G.; Rossi, G.; Degli Esposti, A.; Gazzano, M.; Milita, S.; Bergenti, I.; Ruani, G.; Salitros, I.; Ruben, M.; Cavallini, M.
Surface induces different crystal structures in a room temperature switchable spin crossover compound
Dalton Transactions, (45): 134-143. 2016. 10.1039/c5dt03712c

Geo, M.; Cheng, J. B.; Li, W. Z.; Xiao, B.; Li, Q. Z.
*The aerogen-*pi* bonds involving *pi* systems*
Chemical Physics Letters, (651): 50-55. 2016. 10.1016/j.cplett.2016.03.021

Gericke, R.; Wagler, J.
Ruthenium complexes of diphenylphosphino derivatives of carboxylic amides: Synthesis and characterization of bidentate P,N- and P,O-chelate ligands and their reactivity towards RuCl₂(PPh₃)₃
Polyhedron, (120): 134-141. 2016. 10.1016/j.poly.2016.06.013

Ghadwal, R. S.

Carbon-based two electron sigma-donor ligands beyond classical N-heterocyclic carbenes
Dalton Transactions, (45): 16081-16095. 2016. 10.1039/c6dt02158a

Ghafoori, R.; Ektefa, F.; Zahedi, M.

AlSi2P nanotubes: a theoretical study

Structural Chemistry, (27): 525-533. 2016. 10.1007/s11224-015-0580-1

Ghamsari, P. A.; Nouraliei, M.; Gorgani, S. S.

DFT simulation towards evaluation the molecular structure and properties of the heterogeneous C₁₆Mg₈O₈ nanocage as selective nano-sensor for H-2 and N-2 gases

Journal of Molecular Graphics & Modelling, (70): 163-169. 2016. 10.1016/j.jmgm.2016.08.008

Ghanbarpour, P.; Nori-Shargh, D.

Exploring the origin of the anomeric relationships in 2-cyanoxane, 2-cyanothiane, 2-cyanoselenane and their corresponding isocyano isomers. Correlations between hyper-conjugative anomeric effect, hardness and electrostatic interactions

RSC Advances, (6): 46406-46420. 2016. 10.1039/c6ra06080c

Ghasemi, S.; Noorizadeh, S.

Zero Steric Potential and bond order

Chemical Physics Letters, (652): 106-111. 2016. 10.1016/j.cplett.2016.04.033

Ghasempour, H.; Zakarianezhad, M.; Makiabadi, B.; Habibi-Khorassani, S. M.

Mechanism Investigation of Stable Phosphorus Ylides Derived from Saccharine in the Presence of Different Dialkyl acetylenedicarboxylates: Experimental and Theoretical Study

Iranian Journal of Science and Technology Transaction a-Science, (40): 255-265. 2016. 10.1007/s40995-016-0096-6

Ghashghaei, M.; Ghambarian, M.; Azizi, Z.

Characterization of extraframework Zn²⁺ cationic sites in silicalite-2: a computational study

Structural Chemistry, (27): 467-475. 2016. 10.1007/s11224-015-0575-y

Ghiasi, R.; Manoochehri, M.; Lavasani, R.

DFT and TD-DFT study of benzene and borazines containing chromophores for DSSC materials

Russian Journal of Inorganic Chemistry, (61): 1267-1273. 2016. 10.1134/s0036023616100107

Ghiasi, R.; Nemati, M.; Hakimioun, A. H.

SOLVENT EFFECT ON THE STRUCTURAL, ELECTRONIC, SPECTRA PROPERTIES AND FIRST HYPERPOLARIZABILITY OF W(CO)(5)L, L=(4-PYRIDYL METHYLENE)MALONONITRILE

Journal of the Chilean Chemical Society, (61): 2921-2928. 2016.

Ghiasi, R.; Peikari, A.

Solvent effect on the stability and properties of platinum-substituted borirene and boryl isomers: The polarizable continuum model

Russian Journal of Physical Chemistry A, (90): 2211-2216. 2016. 10.1134/s0036024416110212

Gholipour, A.; Farhadi, S.; Neyband, R. S.

Theoretical investigation of the nature and strength of simultaneous interactions of pi-pi stacking and halogen bond including NMR, SAPT, AIM and NBO analysis

Structural Chemistry, (27): 1543-1551. 2016. 10.1007/s11224-016-0784-z

Gholivand, K.; Asadi, L.; Valmoozi, A. A. E.; Hodaii, M.; Sharifi, M.; Kashani, H. M.; Mahzouni, H. R.; Ghadamayari, M.; Kalate, A. A.; Davari, E.; Salehi, S.; Bonsaii, M.

Phosphorhydrazide inhibitors: toxicological profile and antimicrobial evaluation assay, molecular modeling and QSAR study

RSC Advances, (6): 24175-24189. 2016. 10.1039/c5ra24209f

Gholivand, K.; Farshadfar, K.; Roe, S. M.; Hosseini, M.; Gholami, A.

Investigation of structure-directing interactions within copper(I) thiocyanate complexes through X-ray analyses and non-covalent interaction (NCI) theoretical approach
Crystengcomm, (18): 7104-7115. 2016. 10.1039/c6ce01339b

Gholivand, K.; Farshadfer, K.; Roe, S. M.; Gholami, A.; Esrafili, M. D.
Structural and photophysical characterization of mono- and binuclear Cu(I) complexes based on carbohydrazones: a combined experimental and computational study
Crystengcomm, (18): 2873-2884. 2016. 10.1039/c5ce02208h

Gholivand, K.; Salami, R.; Farshadfar, K.; Butcher, R. J.
Synthesis and structural characterization of Pd(II) and Cu(I) complexes containing dithiophosphorus ligand and their catalytic activities for Heck reaction
Polyhedron, (119): 267-276. 2016. 10.1016/j.poly.2016.09.002

Ghosh, S.; Rahaman, A.; Holt, K. B.; Nordlander, E.; Richmond, M. G.; Kabir, S. E.; Hogarth, G.
Hydrogenase biomimetics with redox-active ligands: Electrocatalytic proton reduction by Fe-2(CO)(4)(kappa(2)-diamine)(mu-edt) (diamine=2,2'-bipy, 1,10-phen)
Polyhedron, (116): 127-135. 2016. 10.1016/j.poly.2016.05.015

Ghosh, S.; Sanchez, B. E.; Richards, I.; Haque, M. N.; Holt, K. B.; Richmond, M. G.; Hogarth, G.
Biomimetics of the FeFe -hydrogenase enzyme: Identification of kinetically favoured apical-basal Fe-2(CO)(4)(mu-H){kappa(2)-Ph2PC(Me-2)}PPh2}{mu-pdt} (+) as a proton-reduction catalyst
Journal of Organometallic Chemistry, (812): 247-258. 2016. 10.1016/j.jorgchem.2015.09.036

Gies, A. P.; Stefanov, Z.; Rau, N. J.; Chakraborty, D.; Boopalachandran, P.; Chauvel, J. P.
Iron(III)-Catalyzed Chain Growth Reactions of Polymeric Methylene Diphenyl Diisocyanate
Macromolecules, (49): 1201-1221. 2016. 10.1021/acs.macromol.5b01973

Giese, T. J.; York, D. M.
Ambient-Potential Composite Ewald Method for ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation
Journal of Chemical Theory and Computation, (12): 2611-2632. 2016. 10.1021/acs.jctc.6b00198

Giesecking, R. L.; Ratner, M. A.; Schatz, G. C.
Implementation of INDO/SCI with COSMO Implicit Solvation and Benchmarking for Solvatochromic Shifts
Journal of Physical Chemistry A, (120): 9878-9885. 2016. 10.1021/acs.jpca.6b10487

Gil, A.; Branchadell, V.; Calhorda, M. J.
A theoretical study of methylation and CH/pi interactions in DNA intercalation: methylated 1,10-phenanthroline in adenine-thymine base pairs
RSC Advances, (6): 85891-85902. 2016. 10.1039/c6ra15495f

Giraldo, C.; Gomez, S.; Weinhold, F.; Restrepo, A.
Insight into the Mechanism of the Michael Reaction
Chemphyschem, (17): 2022-2034. 2016. 10.1002/cphc.201600166

Giri, S.; Inostroza-Rivera, R.; Jana, M.
The Beckmann rearrangement in the framework of reaction electronic flux
Theoretical Chemistry Accounts, (136) 2016. 10.1007/s00214-016-2025-3

Glisic, B. D.; Hoffmann, M.; Warzajtis, B.; Gencic, M. S.; Blagojevic, P. D.; Radulovic, N. S.; Rychlewska, U.; Djuran, W. I.
Selectivity of the complexation reactions of four regioisomeric methylcamphorquinoxaline ligands with gold(III): X-ray, NMR and DFT investigations
Polyhedron, (105): 137-149. 2016. 10.1016/j.poly.2015.12.009

Glisic, B. D.; Savic, N. D.; Warzajtis, B.; Djokic, L.; Ilic-Tomic, T.; Antic, M.; Radenkovic, S.; Nikodinovic-Runic, J.; Rychlewska, U.; Djuran, M. I.

Synthesis, structural characterization and biological evaluation of dinuclear gold(III) complexes with aromatic nitrogen-containing ligands: antimicrobial activity in relation to the complex nuclearity
Medchemcomm, (7): 1356-1366. 2016. 10.1039/c6md00214e

Glushenkov, A. N.; Hovorun, D. M.
Can Nucleobase Pairs Offer a Possibility of a Direct 3D Self-assembly?
Nanoscale Research Letters, (11): 1-7. 2016. 10.1186/s11671-016-1347-3

Gmerek, F.; Stuhlmann, B.; Alvarez-Valtierra, L.; Pratt, D. W.; Schmitt, M.
Electronic spectra of 2-and 3-tolunitrile in the gas phase. II. Geometry changes from Franck-Condon fits of fluorescence emission spectra
Journal of Chemical Physics, (144) 2016. 10.1063/1.4941924

Goettel, J. T.; Gerken, M.
Synthesis and Characterization of Adducts between SF₄ and Oxygen Bases: Examples of O center dot center dot center dot S(IV) Chalcogen Bonding
Inorganic Chemistry, (55): 12441-12450. 2016. 10.1021/acs.inorgchem.6b02373

Goettel, J. T.; Matsumoto, K.; Mercier, H. P. A.; Schrobilgen, G. J.
Syntheses and Structures of Xenon Trioxide Alkylnitrile Adducts
Angewandte Chemie-International Edition, (55): 13780-13783. 2016. 10.1002/anie.201607583

Gokce, H.; Ozturk, N.; Tasan, M.; Alpaslan, Y. B.; Alpaslan, G.
Spectroscopic characterization and quantum chemical computations of the 5-(4-pyridyl)-1H-1,2,4-triazole-3-thiol molecule
Spectroscopy Letters, (49): 167-179. 2016. 10.1080/00387010.2015.1114952

Gold, B.; Aronoff, M. R.; Raines, R. T.
1,3-Dipolar Cycloaddition with Diazo Groups: Noncovalent Interactions Overwhelm Strain
Organic Letters, (18): 4466-4469. 2016. 10.1021/acs.orglett.6b01938

Goldberg, A. R.; Northrop, B. H.
Spectroscopic and Computational Investigations of The Thermodynamics of Boronate Ester and Diazaborole Self-Assembly
Journal of Organic Chemistry, (81): 969-980. 2016. 10.1021/acs.joc.5b02548

Goliaei, A.; Lau, E. Y.; Adhikari, U.; Schwegler, E.; Berkowitz, M. L.
Behavior of P85 and P188 Poloxamer Molecules: Computer Simulations Using United-Atom Force-Field
Journal of Physical Chemistry B, (120): 8631-8641. 2016. 10.1021/acs.jpcb.6b03030

Golub, I. E.; Filippov, O. A.; Belkova, N. V.; Epstein, L. M.; Rossin, A.; Peruzzini, M.; Shubina, E. S.
Two pathways of proton transfer reaction to (triphos)Cu(eta(1)-BH₄) via a dihydrogen bond triphos=1,1,1-tris(diphenylphosphinomethyl)ethane
Dalton Transactions, (45): 9127-9135. 2016. 10.1039/c6dt01104g

Gomez-Pineda, L. E.; Quiroa-Montalvan, C. M.
A COMPUTATIONAL APPROACH TO STUDYING CIPROFLOXACIN AND METHACRYLIC ACID IN PRE-POLYMERIZATION PHASE
Revista Mexicana De Ingenieria Quimica, (15): 667-674. 2016.

Gonthier, J. F.; Sherrill, C. D.
Density-fitted open-shell symmetry-adapted perturbation theory and application to pi-stacking in benzene dimer cation and ionized DNA base pair steps
Journal of Chemical Physics, (145) 2016. 10.1063/1.4963385

Goossens, K.; Lava, K.; Bielawski, C. W.; Binnemans, K.
Ionic Liquid Crystals: Versatile Materials
Chemical Reviews, (116): 4643-4807. 2016. 10.1021/cr400334b

- Gopalsamy, K.; Subramanian, V.
Role of Alkaline Earth Metal Cations in Improving the Hydrogen Storage Capacity of Polyhydroxy Adamantane: A DFT Study
Journal of Physical Chemistry C, (120): 19932-19941. 2016. 10.1021/acs.jpcc.6b03419
- Gopi, R.; Ramanathan, N.; Sundararajan, K.
Blue-shift of the C-H stretching vibration in CHF₃-H₂O complex: Matrix isolation infrared spectroscopy and ab initio computations
Chemical Physics, (476): 36-45. 2016. 10.1016/j.chemphys.2016.07.016
- Gorden, A. E. V.; McKee, M. L.
Computational Study of Reduction Potentials of Th⁴⁺ Compounds and Hydrolysis of ThO₂(H₂O)(n), n=1, 2, 4
Journal of Physical Chemistry A, (120): 8169-8183. 2016. 10.1021/acs.jpca.6b08472
- Gorgani, S. S.; Nouraliei, M.; Gorgani, S. S.
Heterogeneous C₁₆Zn₈O₈ nanocluster as a selective CO/NO nanosensor: computational investigation
International Journal of Environmental Science and Technology, (13): 1573-1580. 2016. 10.1007/s13762-016-0973-8
- Gowda, V.; Laitinen, R. S.; Telkki, V. V.; Larsson, A. C.; Antzutkin, O. N.; Lantto, P.
DFT calculations in the assignment of solid-state NMR and crystal structure elucidation of a lanthanum(III) complex with dithiocarbamate and phenanthroline
Dalton Transactions, (45): 19473-19484. 2016. 10.1039/c6dt03705d
- Gowda, V.; Sarma, B.; Oberg, S.; Telkki, V. V.; Larsson, A. C.; Lantto, P.; Antzutkin, O. N.
Structure Elucidation of an Yttrium Diethyldithiocarbamato-Phenanthroline Complex by X-ray Crystallography, Solid-State NMR, and ab-initio Quantum Chemical Calculations
European Journal of Inorganic Chemistry: 3278-3291. 2016. 10.1002/ejic.201600059
- Goz, V. G.; Pinter, I.; Csampai, A.; Jakli, I.; Zsoldos-Mady, V.; Perczel, A.
Hydrogen-Bonding Network Anchors the Cyclic Form of Sugar Arylhydrazones
European Journal of Organic Chemistry: 3419-3426. 2016. 10.1002/ejoc.201600462
- Grabowski, S. J.
FHF (-) - The Strongest Hydrogen Bond under the Influence of External Interactions
Crystals, (6) 2016. 10.3390/crust6010003
- Grabowski, S. J.; Ruiperez, F.
Dihydrogen bond interactions as a result of H-2 cleavage at Cu, Ag and Au centres
Physical Chemistry Chemical Physics, (18): 12810-12818. 2016. 10.1039/c6cp00046k
- Grabowski, S. J.; Ugalde, J. M.; Andrade, D. M.; Frenking, G.
Comparison of Hydrogen and Gold Bonding in XHX (-), XAuX (-), and Isoelectronic NgHNg (+), NgAuNg (+) (X=Halogen, Ng=Noble Gas)
Chemistry-a European Journal, (22): 11317-11328. 2016. 10.1002/chem.201601392
- Grandner, J. M.; Cacho, R. A.; Tang, Y.; Houk, K. N.
Mechanism of the P450-Catalyzed Oxidative Cyclization in the Biosynthesis of Griseofulvin
ACS Catalysis, (6): 4506-4511. 2016. 10.1021/acscatal.6b01068
- Green, M. L. H.; Parkin, G.
The classification and representation of main group element compounds that feature three-center four-electron interactions
Dalton Transactions, (45): 18784-18795. 2016. 10.1039/c6dt03570a
- Gregson, M.; Lu, E.; Tuna, F.; McInnes, E. J. L.; Hennig, C.; Scheinost, A. C.; McMaster, J.; Lewis, W.; Blake, A. J.; Kerridge, A.; Liddle, S. T.
Emergence of comparable covalency in isostructural cerium(IV)- and uranium(IV)-carbon multiple bonds

Chemical Science, (7): 3286-3297. 2016. 10.1039/c6sc00278a

Greif, A. H.; Hrobarik, P.; Autschbach, J.; Kaupp, M.

Giant spin-orbit effects on H-1 and C-13 NMR shifts for uranium(VI) complexes revisited: role of the exchange-correlation response kernel, bonding analyses, and new predictions

Physical Chemistry Chemical Physics, (18): 30462-30474. 2016. 10.1039/c6cp06129j

Gribanova, T. N.; Minyaev, R. M.; Minkin, V. I.

Stabilization of non-standard conformations of the annulene rings in cyclobutadiene-framed n annulenes (n=8, 10, 12, 14) and their beryllium sandwich-like complexes: a quantum chemical study

Structural Chemistry, (27): 1229-1240. 2016. 10.1007/s11224-016-0748-3

Gribanova, T. N.; Minyaev, R. M.; Minkin, V. I.

Structure and stability of the C-doped boron fullerenes B60C12 and B80C12 with quasi-planar pentacoordinated cage carbon atoms: a quantum-chemical study

Mendeleev Communications, (26): 485-487. 2016. 10.1016/j.mencom.2016.11.008

Grinberg, V. Y.; Tsvetkov, V. B.; Markova, A. A.; Dezhenkova, L. G.; Burova, T. V.; Grinberg, N. V.; Dubovik, A. S.; Plyavnik, N. V.; Shtil, A. A.

Interactions of Non-Phosphorous Glycerolipids with DNA: Energetics, Molecular Docking and Topoisomerase I Attenuation

Anti-Cancer Agents in Medicinal Chemistry, (16): 335-346. 2016. 10.2174/1871520615666150929105907

Gro, L.; Herrmann, C.

GenLocDip: A Generalized Program to Calculate and Visualize Local Electric Dipole Moments

Journal of Computational Chemistry, (37): 2324-2334. 2016. 10.1002/jcc.24420

Groizard, T.; Kahlal, S.; Dorcet, V.; Roisnel, T.; Bruneau, C.; Halet, J. F.; Gramage-Doria, R.

Nonconventional Supramolecular Self-Assemblies of Zinc(II)-Salphen Building Blocks

European Journal of Inorganic Chemistry: 5143-5151. 2016. 10.1002/ejic.201600866

Gronowski, M.; Turowski, M.; Custer, T.; Kolos, R.

A theoretical study on the spectroscopy, structure, and stability of C2H3NS molecules

Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1978-6

Gross, L.; Herrmann, C.

Local electric dipole moments: A generalized approach

Journal of Computational Chemistry, (37): 2260-2265. 2016. 10.1002/jcc.24440

Guan, L.; Li, A. Y.; Song, Y. Y.; Yan, M. Q.; Gao, D. F.; Zhang, X. H.; Li, B.; Wang, L. Y.

Nonplanar Monocyanines: Meso-Substituted Thiazole Orange with High Photostability and Their Synthetic Strategy as well as a Cell Association Study

Journal of Organic Chemistry, (81): 6303-6313. 2016. 10.1021/acs.joc.6b00928

Guevara-Vela, J. M.; Romero-Montalvo, E.; Costales, A.; Pendas, A. M.; Rocha-Rinza, T.

The nature of resonance-assisted hydrogen bonds: a quantum chemical topology perspective

Physical Chemistry Chemical Physics, (18): 26383-26390. 2016. 10.1039/c6cp04386k

Guevara-Vela, J. M.; Romero-Montalvo, E.; Gomez, V. A. M.; Chavez-Calvillo, R.; Garcia-Revilla, M.; Francisco, E.; Pendas, A. M.; Rocha-Rinza, T.

Hydrogen bond cooperativity and anticooperativity within the water hexamer

Physical Chemistry Chemical Physics, (18): 19557-19566. 2016. 10.1039/c6cp00763e

Guin, M.; Nayak, A. N.; Gowda, N. M. M.

Theoretical study of hydrogen bonded picolinic acid-water complexes

Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (55): 782-792. 2016.

- Gumbau-Brisa, R.; Hayward, J. J.; Wallis, J. D.; Rawson, J. M.; Pilkington, M.
Structural insights into the coordination chemistry and reactivity of a 3,3'-bis-imine-2,2'-bipyridine ligand
CrystEngComm, (18): 1892-1903. 2016. 10.1039/c5ce02349a
- Gumus, H. P.; Tamer, O.; Avci, D.; Atalay, Y.
Density functional theory calculations on conformational, spectroscopic and electrical properties of 3-(2,3-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one: a potential nonlinear optical material
Indian Journal of Physics, (90): 79-89. 2016. 10.1007/s12648-015-0730-8
- Gumus, H. P.; Tamer, O.; Avci, D.; Atalay, Y.; Tarcan, E.
A Theoretical Study on Structural, Spectroscopic, Electronic and Nonlinear Optical Properties of 1-(E)-{4-(Morpholin-4-Yl)Phenyl Imino}Methyl Naphthalen-2-Ol
Brazilian Journal of Physics, (46): 471-480. 2016. 10.1007/s13538-016-0432-5
- Gunay, N.; Tamer, O.; Kuzalic, D.; Avci, D.; Atalay, Y.
Synthesis, spectroscopic characterization and DFT calculations on N-(Phenylsulfonyl)-L-asparagine (NPLAS): A potential nonlinear optical material
Optik, (127): 8782-8794. 2016. 10.1016/j.ijleo.2016.06.087
- Guo, J. Y.; Chai, H. Y.; Duan, Q.; Qin, J. M.; Shen, X. D.; Jiang, D. Y.; Hou, J. H.; Yan, B.; Li, Z. R.; Gu, F. L.; Li, Q. S.
Planar tetracoordinate carbon species Cl₃E with 12-valence-electrons
Physical Chemistry Chemical Physics, (18): 4589-4593. 2016. 10.1039/c5cp06081h
- Guo, X.; Yang, Y. P.; Li, Q. Z.; Li, H. B.
Origin of selenium-gold interaction in F₂CSe center dot center dot center dot AuY (Y = CN, F, Cl, Br, OH, and CH₃): Synergistic effects
Journal of Chemical Physics, (144) 2016. 10.1063/1.4944088
- Guo, X. J.; Xiong, X. G.; Li, C.; Gong, H. F.; Huai, P.; Hu, J. T.; Jin, C.; Huang, L. L.; Wu, G. Z.
DFT investigations of uranium complexation with amidoxime-, carboxyl- and mixed amidoxime/carboxyl-based host architectures for sequestering uranium from seawater
Inorganica Chimica Acta, (441): 117-125. 2016. 10.1016/j.ica.2015.11.013
- Gupta, N. K.; Sengupta, A.; Boda, A.; Adya, V. C.; Ali, S. M.
Oxidation state selective sorption behavior of plutonium using N, N-dialkylamide functionalized carbon nanotubes: experimental study and DFT calculation
RSC Advances, (6): 78692-78701. 2016. 10.1039/c6ra17773e
- Gupta, R.; Bansal, R. K.
Aromaticity/antiaromaticity of phospha-analogues of carbocyclic ions: A DFT investigation
Computational and Theoretical Chemistry, (1076): 1-10. 2016. 10.1016/j.comptc.2015.11.020
- Gutsev, G. L.; Belay, K. G.; Bozhenko, K. V.; Gutsev, L. G.; Ramachandran, B. R.
A comparative study of small 3d-metal oxide (FeO)(n), (CoO)(n), and (NiO)(n) clusters
Physical Chemistry Chemical Physics, (18): 27858-27867. 2016. 10.1039/c6cp03241a
- Gutsev, G. L.; Belay, K. G.; Gutsev, L. G.; Ramachandran, B. R.
Structure and Properties of Iron Oxide Clusters: From Fe-6 to Fe₆O₂₀ and from Fe-7 to Fe₇O₂₄
Journal of Computational Chemistry, (37): 2527-2536. 2016. 10.1002/jcc.24478
- Gutsev, L. G.; Dalal, N. S.; Maroulis, G.; Gutsev, G. L.
Structure and magnetic properties of Cd_{9-n}Se₉M_n and Cd_{9-n}Se₉F_n clusters (n=0-9)
Chemical Physics, (469): 105-114. 2016. 10.1016/j.chemphys.2016.02.008
- Guveli, S.; Cinar, S. A.; Karahan, O.; Aviyente, V.; Ulkuseven, B.
Nickel(II)-PPh₃ Complexes of S,N-Substituted Thiosemicarbazones - Structure, DFT Study, and Catalytic Efficiency
European Journal of Inorganic Chemistry: 538-544. 2016. 10.1002/ejic.201501227

- Gyepes, R.; Pinkas, J.; Cisarova, I.; Kubista, J.; Horacek, M.; Mach, K.
Synthesis, molecular and electronic structure of a stacked half-sandwich dititanium complex incorporating a cyclic pi-faced bridging ligand
RSC Advances, (6): 94149-94159. 2016. 10.1039/c6ra14940e
- Hagar, M.; Soliman, S. M.; Ibid, F.; El Ashry, E. H.
Synthesis, molecular structure and spectroscopic studies of some new quinazolin-4(3H)-one derivatives; an account on the N- versus S-Alkylation
Journal of Molecular Structure, (1108): 667-679. 2016. 10.1016/j.molstruc.2015.12.007
- Haghdadi, M.; Abaszade, A.; Abadian, L.; Nab, N.; Bosra, H. G.
A theoretical study on the hetero-Diels-Alder reaction of phosphorous substituted diaza- and oxaza-alkenes with olefins derivatives
RSC Advances, (6): 89440-89449. 2016. 10.1039/c6ra15496d
- Haghdadi, M.; Moradi, A.; Bosra, H. G.
DFT study on the mechanism of the Diels-Alder reactions leading to bicyclo 4.2.0 octenones
Progress in Reaction Kinetics and Mechanism, (41): 67-75. 2016. 10.3184/146867816x14506899861213
- Haghdadi, M.; Mousavi, S. S.; Ghasemnejad, H.
Stepwise or concerted? A DFT study on the mechanism of ionic Diels-Alder reactions of chromanes
Journal of the Serbian Chemical Society, (81): 67-80. 2016. 10.2298/jsc150420089h
- Haghdadi, M.; Nab, N.; Bosra, H. G.
DFT study on the regio- and stereo-selectivity of the Diels-Alder reaction between a cycloprop-2-ene carboxylate and some cyclic 1,3-dienes
Progress in Reaction Kinetics and Mechanism, (41): 193-204. 2016. 10.3184/146867816x14636767119354
- Haines, B. E.; Berry, J. F.; Yu, J. Q.; Musaey, D. G.
Factors Controlling Stability and Reactivity of Dimeric Pd(II) Complexes in C-H Functionalization Catalysis
ACS Catalysis, (6): 829-839. 2016. 10.1021/acscatal.5b02447
- Hajibabadi, H.; Nowroozi, A.
Study on the interaction of metallocene catalysts with the surface of carbon nanotubes and its influence on the catalytic properties. 1. Investigation of possible complex structures and the influence on structural and electronic properties
Journal of Organometallic Chemistry, (818): 154-162. 2016. 10.1016/j.jorgchem.2016.06.016
- Halbert, S.; Coperet, C.; Raynaud, C.; Eisenstein, O.
Elucidating the Link between NMR Chemical Shifts and Electronic Structure in d(0) Olefin Metathesis Catalysts
Journal of the American Chemical Society, (138): 2261-2272. 2016. 10.1021/jacs.5b12597
- Hale, L. V. A.; Malakar, T.; Tseng, K. N. T.; Zimmerman, P. M.; Paul, A.; Szymczak, N. K.
The Mechanism of Acceptorless Amine Double Dehydrogenation by N,N,N-Amide Ruthenium(II) Hydrides: A Combined Experimental and Computational Study
ACS Catalysis, (6): 4799-4813. 2016. 10.1021/acscatal.6b01465
- Halim, M. A.; Girod, M.; MacAleese, L.; Lemoine, J.; Antoine, R.; Dugourd, P.
213 nm Ultraviolet Photodissociation on Peptide Anions: Radical-Directed Fragmentation Patterns
Journal of the American Society for Mass Spectrometry, (27): 474-486. 2016. 10.1007/s13361-015-1297-5
- Hallooman, D.; Rios-Gutierrez, M.; Rhyman, L.; Alswaidan, I. A.; Fun, H. K.; Domingo, L. R.; Ramasami, P.
3+2 Cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl acrylate: A DFT study
Computational and Theoretical Chemistry, (1087): 36-47. 2016. 10.1016/j.comptc.2016.04.015
- Hamdaoui, M.; Ney, M.; Sarda, V.; Karmazin, L.; Bailly, C.; Sieffert, N.; Dohm, S.; Hansen, A.; Grimme, S.; Djukic, J. P.
Evidence of a Donor-Acceptor (Ir-H)-> SiR3 Interaction in a Trapped Ir(III) Silane Catalytic Intermediate

Organometallics, (35): 2207-2223. 2016. 10.1021/acs.organomet.6b00248

Han, C. L.; Dong, Y. Y.; Wang, B. Q.; Zhang, C. Y.

Ca(BH₄)₂(n) Clusters As Hydrogen Storage Material: A DFT Study

Russian Journal of Physical Chemistry A, (90): 1997-2005. 2016. 10.1134/s0036024416100071

Haner, J.; Matsumoto, K.; Mercier, H. P. A.; Schrobilgen, G. J.

Nature of the Xe-VI-N Bonds in F₆XeNCCH₃ and F₆Xe(NCCH₃)₂ and the Stereochemical Activity of Their Xenon Valence Electron Lone Pairs

Chemistry-a European Journal, (22): 4833-4842. 2016. 10.1002/chem.201504904

Hansen, E.; Lime, E.; Norrby, P. O.; Wiest, O.

Anomeric Effects in Sulfamides

Journal of Physical Chemistry A, (120): 3677-3682. 2016. 10.1021/acs.jpca.6b02757

Hao, J. J.; Rheingold, A. L.; Kavand, M.; van Schooten, K. J.; Boehme, C.; Capdevila-Cortada, M.; Novoa, J. J.; Woss, E.; Knor, G.; Miller, J. S.

The Tetracyanopyridinide Dimer Dianion, sigma- TCNPy (2)(2-)

Chemistry-a European Journal, (22): 12312-12315. 2016. 10.1002/chem.201603071

Haress, N. G.; Manimaran, D.; Joe, I. H.; El-Azzouny, A. A.; Al-Wabli, R. I.; Attia, M. I.

Vibrational and electronic profiles, molecular docking and biological prediction of 5-methoxy-1- (5-methoxy-1H-indol-2-yl) methyl -1H-indole: Experimental and theoretical investigations

Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500462

Harris, M.; Brusey, S. A.; Moore, A.; Ortin, Y.; Muller-Bunz, H.; Manca, G.; Mealli, C.; McGlinchey, M. J.

Co-2(CO)(6)(Alkynyl) Complexes of Dibenzosuberyl and Dibenzosuberanyl Carbocations: Dibenzotropylium or Dibenzoheptafulvene?

Chempluschem, (81): 292-306. 2016. 10.1002/cplu.201500477

Harris, T.; Gomes, G. D.; Clark, R. J.; Alabugin, I. V.

Domino Fragmentations in Traceless Directing Groups of Radical Cascades: Evidence for the Formation of Alkoxy Radicals via C-O Scission

Journal of Organic Chemistry, (81): 6007-6017. 2016. 10.1021/acs.joc.6b01052

Harrison, J. A.; Nielson, A. J.; Sajjad, M. A.; Saunders, G. C.; Schwerdtfeger, P.

Steric and Electronic Manipulation of the Anagostic Interaction in 1-Tetralone Oxime and Imine Complexes of Rhodium(I)

European Journal of Inorganic Chemistry: 64-77. 2016. 10.1002/ejic.201501122

Harrison, J. A.; Sajjad, M. A.; Schwerdtfeger, P.; Nielson, A. J.

Multiple Weak C-H Intramolecular Hydrogen Bonding as an Aid to Minimizing Bond Rotation Flexibility

Crystal Growth & Design, (16): 4934-4942. 2016. 10.1021/acs.cgd.6b00496

Haruna, K.; Alenaizan, A. A.; Al-Saadi, A. A.

Density functional theory study of the substituent effect on the structure, conformation and vibrational spectra in halosubstituted anilines

RSC Advances, (6): 67794-67804. 2016. 10.1039/c6ra11908e

Haruna, K.; Saleh, T. A.; Al Thagfi, J.; Al-Saadi, A. A.

Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: A comparative study

Journal of Molecular Structure, (1121): 7-15. 2016. 10.1016/j.molstruc.2016.05.021

Hasegawa, J.; Miyazaki, R.; Maeda, C.; Ema, T.

Theoretical Study on Highly Active Bifunctional Metalloporphyrin Catalysts for the Coupling Reaction of Epoxides with Carbon Dioxide

Chemical Record, (16): 2260-2267. 2016. 10.1002/tcr.201600053

- Hashemi, M.
Comparison of reactivity of Pt(II) center in the mononuclear and binuclear organometallic diimineplatinum complexes toward oxidative addition of methyl iodide
Journal of Molecular Structure, (1103): 132-139. 2016. 10.1016/j.molstruc.2015.09.017
- Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y.
Water Entrapped inside Fullerene Cages: A Potential Probe for Evaluation of Bond Polarization
Angewandte Chemie-International Edition, (55): 13109-13113. 2016. 10.1002/anie.201607040
- Hauser, A. W.; Horn, P. R.; Head-Gordon, M.; Bell, A. T.
A systematic study on Pt based, subnanometer-sized alloy cluster catalysts for alkane dehydrogenation: effects of intermetallic interaction
Physical Chemistry Chemical Physics, (18): 10906-10917. 2016. 10.1039/c6cp00360e
- He, F.; Yang, X.; Tian, Z. Y.; Wang, H. G.; Xue, Y.
Theoretical investigation on the structures and bonding properties of Pd(II), Pt(II) and Ni(II) complexes with tridentate CNC-pincer N-heterocyclic carbene ligands
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500371
- He, H. M.; Li, Y.; Sun, W. M.; Wang, J. J.; Wu, D.; Zhong, R. L.; Zhou, Z. J.; Li, Z. R.
All-metal electride molecules CuAg@Ca7M (M = Be, Mg, and Ca) with multi-excess electrons and all-metal polyanions: molecular structures and bonding modes as well as large infrared nonlinear optical responses
Dalton Transactions, (45): 2656-2665. 2016. 10.1039/c5dt04530d
- He, K. D.; Allen, W. D.
Conformers of Gaseous Serine
Journal of Chemical Theory and Computation, (12): 3571-3582. 2016. 10.1021/acs.jctc.6b00314
- He, N.; Li, Z. H.
Palladium-atom catalyzed formic acid decomposition and the switch of reaction mechanism with temperature
Physical Chemistry Chemical Physics, (18): 10005-10017. 2016. 10.1039/c6cp00186f
- He, W. X.; Tan, X. J.; Wang, N. N.; Zhang, H.
Theoretical study on the mechanism of the cycloaddition reaction between ketenimine and hydrogen cyanide
Journal of the Serbian Chemical Society, (81): 187-195. 2016. 10.2298/jsc150504091h
- He, Y. H.; Zhou, L. X.
A theoretical study on pyridine gold (III) complexes AuCl₃ (Hpm) and AuCl₂ (pm) targeting purine bases and cysteine
Computational and Theoretical Chemistry, (1093): 20-28. 2016. 10.1016/j.comptc.2016.08.008
- Heggen, B.; Patil, M.; Thiel, W.
Cyclization of an alpha,beta-Unsaturated Hydrazone Catalyzed by a BINOL-Phosphoric Acid: Pericyclic or Not?
Journal of Computational Chemistry, (37): 280-285. 2016. 10.1002/jcc.24044
- Hejazi, S. A.; Osman, O. I.; Alyoubi, A. O.; Aziz, S. G.; Hilal, R. H.
The Thermodynamic and Kinetic Properties of 2-Hydroxypyridine/2-Pyridone Tautomerization: A Theoretical and Computational Revisit
International Journal of Molecular Sciences, (17) 2016. 10.3390/ijms17111893
- Henkel, S.; Costa, P.; Klute, L.; Sokkar, P.; Fernandez-Oliva, M.; Thiel, W.; Sanchez-Garcia, E.; Sander, W.
Switching the Spin State of Diphenylcarbene via Halogen Bonding
Journal of the American Chemical Society, (138): 1689-1697. 2016. 10.1021/jacs.5b12726
- Henrion, S.; Carboni, B.; Cossio, F. P.; Roisnel, T.; Villalgordo, J. M.; Carreaux, F.
Stereospecific Synthesis of alpha-Amino Allylsilane Derivatives through a 3,3 -Allyl Cyanate Rearrangement. Mild Formation of Functionalized Disiloxanes
Journal of Organic Chemistry, (81): 4633-4644. 2016. 10.1021/acs.joc.6b00505

- Herrera, R.; Mendez, F.; Jimenez, F.; Cruz, M. C.; Tamariz, J.
Theoretical study of the regioselective cyclization of enaminones in the construction of benzofurans and indoles
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2985-1
- Heshmatipour, F.; Beyramabadi, S. A.; Morsali, A.; Heravi, M. M.
A DFT study on the geometry, spectroscopic properties, and tautomerization of the local anaesthetic drug prilocaine
Journal of Structural Chemistry, (57): 1096-1103. 2016. 10.1134/s0022476616060068
- Hesselmann, A.
Local Molecular Orbitals from a Projection onto Localized Centers
Journal of Chemical Theory and Computation, (12): 2720-2741. 2016. 10.1021/acs.jctc.6b00321
- Hester, T. H.; Albury, R. M.; Pruitt, C. J. M.; Goebbert, D. J.
Fragmentation of Ni(NO₃)₃(-) : A Study of Nickel-Oxygen Bonding and Oxidation States in Nickel Oxide Fragments
Inorganic Chemistry, (55): 6634-6642. 2016. 10.1021/acs.inorgchem.6b00812
- Hester, T. H.; Goebbert, D. J.
Experimental and theoretical study of the decomposition of Zn(NO₃)₃(-)
Chemical Physics Letters, (660): 277-282. 2016. 10.1016/j.cplett.2016.08.039
- Hinz, A.; Goicoechea, J. M.
A Monoanionic Arsenide Source: Decarbonylation of the 2-Arsaethynolate Anion upon Reaction with Bulky Stannylenes
Angewandte Chemie-International Edition, (55): 15515-15519. 2016. 10.1002/anie.201609309
- Hinz, A.; Rothe, J.; Schulz, A.; Villinger, A.
Reduction of dichloro(diaza-phospho)stibanes - isolation of a donor-stabilized distibenium dication
Dalton Transactions, (45): 6044-6052. 2016. 10.1039/c5dt02711j
- Hinz, A.; Schulz, A.; Villinger, A.
Synthesis of a Molecule with Four Different Adjacent Pnictogens
Chemistry-a European Journal, (22): 12266-12269. 2016. 10.1002/chem.201601916
- Hirai, M.; Cho, J. S.; Gabbai, F. P.
Promoting the Hydrosilylation of Benzaldehyde by Using a Dicationic Antimony-Based Lewis Acid: Evidence for the Double Electrophilic Activation of the Carbonyl Substrate
Chemistry-a European Journal, (22): 6537-6541. 2016. 10.1002/chem.201600971
- Hiraide, S.; Tanaka, H.; Miyahara, M. T.
Understanding gate adsorption behaviour of CO₂ on elastic layer-structured metal-organic framework-11
Dalton Transactions, (45): 4193-4202. 2016. 10.1039/c5dt03476k
- Hirshberg, B.; Gerber, R. B.
Formation of Carbonic Acid in Impact of CO₂ on Ice and Water
Journal of Physical Chemistry Letters, (7): 2905-2909. 2016. 10.1021/acs.jpcllett.6b01109
- Hlina, J. A.; Pankhurst, J. R.; Kaltsoyannis, N.; Arnold, P. L.
Metal-Metal Bonding in Uranium-Group 10 Complexes
Journal of the American Chemical Society, (138): 3333-3345. 2016. 10.1021/jacs.5b10698
- Hobza, P.; Rezac, J.
Introduction: Noncovalent Interactions
Chemical Reviews, (116): 4911-4912. 2016. 10.1021/acs.chemrev.6b00247
- Hoffmann, A.; Herres-Pawlis, S.
Donor-driven conformational flexibility in a real-life catalytic dicopper(II) peroxy complex
Physical Chemistry Chemical Physics, (18): 6430-6440. 2016. 10.1039/c5cp05009j

Hoffmann, A.; Stanek, J.; Dicke, B.; Peters, L.; Grimm-Lebsanft, B.; Wetzel, A.; Jesser, A.; Bauer, M.; Gnida, M.; Meyer-Klaucke, W.; Rubhausen, M.; Herres-Pawlis, S.

Implications of Guanidine Substitution on Copper Complexes as Entatic-State Models
European Journal of Inorganic Chemistry: 4731-4743. 2016. 10.1002/ejic.201600655

Hoffmann, R.; Alvarez, S.; Mealli, C.; Falceto, A.; Cahill, T. J.; Zeng, T.; Manca, G.

From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields
Chemical Reviews, (116): 8173-8192. 2016. 10.1021/acs.chemrev.6b00251

Hokmabady, L.; Raissi, H.; Khanmohammadi, A.

Interactions of the 5-fluorouracil anticancer drug with DNA pyrimidine bases: a detailed computational approach
Structural Chemistry, (27): 487-504. 2016. 10.1007/s11224-015-0578-8

Holler, S.; Tuchler, M.; Belaj, F.; Veiros, L. F.; Kirchner, K.; Mosch-Zanetti, N. C.

Thiopyridazine-Based Copper Boratrane Complexes Demonstrating the Z-type Nature of the Ligand
Inorganic Chemistry, (55): 4980-4991. 2016. 10.1021/acs.inorgchem.6b00464

Hollering, M.; Reithmeier, R. O.; Meister, S.; Herdtweck, E.; Kuhn, F. E.; Rieger, B.

Re(CO)(3)Cl(C5H4ClP)(2) and Re(CO)(2)Cl(C5H4ClP)(3) : synthesis and characterization of two novel rhenium(I) phosphinine complexes
RSC Advances, (6): 14134-14139. 2016. 10.1039/c5ra25904e

Hollmann, K.; Oppermann, A.; Amen, M.; Florke, U.; Egold, H.; Hoffmann, A.; Herres-Pawlis, S.; Henkel, G.

Addressing Hydrogen Bonding Motifs by Suited Substitution of Thioureas
Zeitschrift fur Anorganische und Allgemeine Chemie, (642): 660-669. 2016. 10.1002/zaac.201600126

Horn, P. R.; Head-Gordon, M.

Alternative definitions of the frozen energy in energy decomposition analysis of density functional theory calculations
Journal of Chemical Physics, (144) 2016. 10.1063/1.4941849

Horn, P. R.; Mao, Y. Z.; Head-Gordon, M.

Defining the contributions of permanent electrostatics, Pauli repulsion, and dispersion in density functional theory calculations of intermolecular interaction energies
Journal of Chemical Physics, (144) 2016. 10.1063/1.4942921

Horn, P. R.; Mao, Y. Z.; Head-Gordon, M.

Probing non-covalent interactions with a second generation energy decomposition analysis using absolutely localized molecular orbitals
Physical Chemistry Chemical Physics, (18): 23067-23079. 2016. 10.1039/c6cp03784d

Hosseini, F. N.; Rashidi, M.; Nabavizadeh, S. M.

Synthesis of diorganoplatinum(IV) complexes by the S-S bond cleavage with platinum(II) complexes
Journal of Molecular Structure, (1125): 20-26. 2016. 10.1016/j.molstruc.2016.06.049

Hosseini, S.; Nori-Shargh, D.

Exploring the structural and conformational properties of dioxygen dihalides (halogen = F, Cl, Br)
Canadian Journal of Chemistry, (94): 176-187. 2016. 10.1139/cjc-2015-0399

Hou, X. F.; Yan, L. L.; Huang, T.; Hong, Y.; Miao, S. K.; Peng, X. Q.; Liu, Y. R.; Huang, W.

A density functional theory study on structures, stabilities, and electronic and magnetic properties of AunC ($n=1-9$) clusters
Chemical Physics, (472): 50-60. 2016. 10.1016/j.chemphys.2016.03.009

Houston, S. A.; Venkataraman, N. S.; Suvitha, A.; Wheate, N. J.

Loading of a Phenanthroline-Based Platinum(II) Complex onto the Surface of a Carbon Nanotube via pi-pi Stacking
Australian Journal of Chemistry, (69): 1124-1129. 2016. 10.1071/ch16067

Hoyvik, I. M.; Jorgensen, P.

Characterization and Generation of Local Occupied and Virtual Hartree-Fock Orbitals
Chemical Reviews, (116): 3306-3327. 2016. 10.1021/acs.chemrev.5b00492

Hsu, W.; Thapa, K. B.; Yang, X. K.; Chen, K. T.; Chang, H. Y.; Chen, J. D.
Dinitrogen-supported coordination polymers
CrystEngComm, (18): 390-393. 2016. 10.1039/c5ce02127h

Hu, K. Q.; Zhu, L. Z.; Wang, C. Z.; Mei, L.; Liu, Y. H.; Gao, Z. Q.; Chai, Z. F.; Shi, W. Q.
Novel Uranyl Coordination Polymers Based on Quinoline-Containing Dicarboxylate by Altering Auxiliary Ligands: From 1D Chain to 3D Framework
Crystal Growth & Design, (16): 4886-4896. 2016. 10.1021/acs.cgd.6b00429

Hu, S. X.; Gibson, J. K.; Li, W. L.; Van Stipdonk, M. J.; Martens, J.; Berden, G.; Redlich, B.; Oomens, J.; Li, J.
Electronic structure and characterization of a uranyl di-15-crown-5 complex with an unprecedented sandwich structure
Chemical Communications, (52): 12761-12764. 2016. 10.1039/c6cc07205d

Huang, S.; Yang, B. Z.; Ren, A. M.
Theoretical investigation on ratiometric two-photon fluorescent probe for Zn²⁺ detection based on ICT mechanism
Journal of Molecular Structure, (1114): 65-77. 2016. 10.1016/j.molstruc.2016.02.055

Huang, S. Y.; Liao, K. T.; Peng, B.; Luo, Q.
On the Potential of Using the Al-7 Superatom as an Excess Electron Acceptor To Construct Materials with Excellent Nonlinear Optical Properties
Inorganic Chemistry, (55): 4421-4427. 2016. 10.1021/acs.inorgchem.6b00224

Huang, W.; Xu, W. H.; Schwarz, W. H. E.; Li, J.
On the Highest Oxidation States of Metal Elements in MO₄ Molecules (M = Fe, Ru, Os, Hs, Sm, and Pu)
Inorganic Chemistry, (55): 4616-4625. 2016. 10.1021/acs.inorgchem.6b00442

Huang, X. C.; Wang, H. F.; Lang, J. P.
Theoretical view on a linear end-on manganese-dioxygen complex bearing a calix 4 arene ligand
RSC Advances, (6): 81517-81526. 2016. 10.1039/c6ra11199h

Huang, Y. J.; Pa, Y. R.; Du, G.; Ca, Y. X.
Extended structures of two coordination polymers based on 1,10-phenanthroline derivatives: Preparation, structural characterization and properties
Journal of Chemical Sciences, (128): 459-465. 2016. 10.1007/s12039-016-1035-y

Huang, Y. J.; Pan, Y. R.; Dong, Y.
Hydrothermal Synthesis, Characterization, and Natural Bond Orbital Analysis of a Complex With Pyridinedicarboxylic Acid and N-Donor Ligand: 2-Methyldipyrido 3,2-f:2',3'-h quinoxaline
Synthesis and Reactivity in Inorganic Metal-Organic and Nano-Metal Chemistry, (46): 908-912. 2016.
10.1080/15533174.2014.989609

Hudson, B. M.; Nguyen, E.; Tantillo, D. J.
The influence of intramolecular sulfur-lone pair interactions on small-molecule drug design and receptor binding
Organic & Biomolecular Chemistry, (14): 3975-3980. 2016. 10.1039/c6ob00254d

Hyodo, K.; Nishihara, Y.
Highly Selective Synthesis of Multi-substituted Olefins Mediated by Zirconocene Complexes
Journal of Synthetic Organic Chemistry Japan, (74): 792-802. 2016. 10.5059/yukigoseikyokaishi.74.792

Ignatyev, I. S.; Montejo, M.; Ortega, P. G. R.; Kochina, T. A.; Gonzalez, J. J. L.
DFT study of the hydrolysis reaction in atraanes and ocanes: the influence of transannular bonding
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-015-2880-1

Imura, T.; Akasaka, N.; Iwamoto, T.

A Dialkylsilylene-Pt(0) Complex with a DVTMS Ligand for the Catalytic Hydrosilylation of Functional Olefins
Organometallics, (35): 4071-4076. 2016. 10.1021/acs.organomet.6b00741

Illan-Cabeza, N. A.; Jimenez-Pulido, S. B.; Hueso-Urena, F.; Pena-Ruiz, T.; Quiros-Olozabal, M.; Moreno-Carretero, M. N.
Interactions between 2,4-bis-pteridine-1,5-benzodiazepine and group 12 dihalides: synthesis, spectral and XRD structural studies and theoretical calculations
Dalton Transactions, (45): 17896-17909. 2016. 10.1039/c6dt03583c

Ioannidis, E. I.; Gani, T. Z. H.; Kulik, H. J.
molSimplify: A toolkit for automating discovery in inorganic chemistry
Journal of Computational Chemistry, (37): 2106-2117. 2016. 10.1002/jcc.24437

Iramain, M. A.; Davies, L.; Brandan, S. A.
FTIR, HATR and FT-Raman studies on the anhydrous and monohydrate species of maltose in aqueous solution
Carbohydrate Research, (428): 41-56. 2016. 10.1016/j.carres.2016.04.013

Irani, M.; Mohammadi, T.; Mohebbi, S.
Photocatalytic Degradation of Methylene Blue with ZnO Nanoparticles; a Joint Experimental and Theoretical Study
Journal of the Mexican Chemical Society, (60): 218-225. 2016.

Isaev, A. N.
Hydrogen bonded D-H center dot center dot center dot Y (Y = O, S, Hal) molecular complexes: A natural bond orbital analysis
Russian Journal of Physical Chemistry A, (90): 601-609. 2016. 10.1134/s0036024416030183

Isaev, A. N.
Intermolecular charge transfer as evidence for unusual O-H center dot center dot center dot C(sp³) hydrogen bond
Computational and Theoretical Chemistry, (1090): 180-192. 2016. 10.1016/j.comptc.2016.06.014

Isaev, A. N.
O-H center dot center dot center dot C Hydrogen Bond in the Methane-Water Complex
Russian Journal of Physical Chemistry A, (90): 1978-1985. 2016. 10.1134/s0036024416100150

Ishii, T.; Suzuki, K.; Nakamura, T.; Yamashita, M.
An Isolable Bismabenzeno: Synthesis, Structure, and Reactivity
Journal of the American Chemical Society, (138): 12787-12790. 2016. 10.1021/jacs.6b08714

Ishitsuka, T.; Okuda, Y.; Szilagyi, R. K.; Mori, S.; Nishihara, Y.
The molecular mechanism of palladium-catalysed cyanoesterification of methyl cyanoformate onto norbornene
Dalton Transactions, (45): 7786-7793. 2016. 10.1039/c6dt00341a

Ismail, I.; Okajima, T.; Kawauchi, S.; Ohsaka, T.
Studies on the early oxidation process of dopamine by electrochemical measurements and quantum chemical calculations
Electrochimica Acta, (211): 777-786. 2016. 10.1016/j.electacta.2016.05.056

Ivanov, A. S.; Kar, T.; Boldyrev, A. I.
Nanoscale stabilization of zintl compounds: 1D ionic Li-P double helix confined inside a carbon nanotube
Nanoscale, (8): 3454-3460. 2016. 10.1039/c5nr07713c

Ivanov, D. M.; Kirina, Y. V.; Novikov, A. S.; Starova, G. L.; Kukushkin, V. Y.
Efficient pi-stacking with benzene provides 2D assembly of trans- PtCl₂(p-CF₃C₆H₄CN)(2)
Journal of Molecular Structure, (1104): 19-23. 2016. 10.1016/j.molstruc.2015.09.027

Iyasamy, S.; Varadharajan, K.; Sivagnanam, S.
Density Functional Theory Calculations, Spectroscopic (FT-IR, FT-RAMAN), Frontier Molecular Orbital, Molecular Electrostatic Potential Analysis of 5-Fluoro-2-Methylbenzaldehyde

Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics, (230): 1681-1710. 2016. 10.1515/zpch-2016-0839

Jaeger, B. K. A.; Savoca, M.; Dopfer, O.; Truong, N. X.

Photodissociation spectrum and structure of Au-4(+)center dot H2O clusters

International Journal of Mass Spectrometry, (402): 49-56. 2016. 10.1016/j.ijms.2016.02.019

Jafari, S.; Ryde, U.; Irani, M.

Catalytic mechanism of human glyoxalase I studied by quantum-mechanical cluster calculations

Journal of Molecular Catalysis B-Enzymatic, (131): 18-30. 2016. 10.1016/j.molcatb.2016.05.010

Jako, S.; Lupan, A.; Kun, A. Z.; King, R. B.

Polyhedral dinickelaboranes as analogues of the dicarbaboranes

Polyhedron, (110): 31-36. 2016. 10.1016/j.poly.2016.02.016

Jalife, S.; Mondal, S.; Cabellos, J. L.; Pan, S.; Mendez-Rojas, M. A.; Fernandez, I.; Frenking, G.; Merino, G.

Breaking the Isolated Pentagon Rule by Encapsulating Xe-2 in C-60: The Guest Defines the Shape of the Host

Chemistryselect, (1): 2405-2408. 2016. 10.1002/slct.201600525

Jambrec, D.; Haddad, R.; Lauks, A.; Gebala, M.; Schuhmann, W.; Kokoschka, M.

DNA Intercalators for Detection of DNA Hybridisation: SCS(MI)-MP2 Calculations and Electrochemical Impedance Spectroscopy

Chempluschem, (81): 604-612. 2016. 10.1002/cplu.201600173

Jamshidi, M.; Nematollahi, D.; Bayat, M.; Salahifar, E.

Unsymmetrical Diaryl Sulfones through Electrochemical Oxidation of Fast Violet B in the Presence of Aryl Sulfinic Acids

Journal of the Electrochemical Society, (163): G211-G218. 2016. 10.1149/2.1431614jes

Jana, G.; Saha, R.; Pan, S.; Kumar, A.; Merino, G.; Chattaraj, P. K.

Noble Gas Binding Ability of Metal-Bipyridine Monocationic Complexes (Metal=Cu, Ag, Au): A Computational Study

Chemistryselect, (1): 5842-5849. 2016. 10.1002/slct.201601245

Janesko, B. G.

Topological analysis of the electron delocalization range

Journal of Computational Chemistry, (37): 1993-2005. 2016. 10.1002/jcc.24421

Janesko, B. G.; Wiberg, K. B.; Scalmani, G.; Frisch, M. J.

Electron Delocalization Range in Atoms and on Molecular Surfaces

Journal of Chemical Theory and Computation, (12): 3185-3194. 2016. 10.1021/acs.jctc.6b00343

Jasik, M.; Szefczyk, B.

Parameterization and optimization of the menthol force field for molecular dynamics simulations

Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3082-1

Jasmine, G. F.; Amalanathan, M.; Roy, S. D. D.

Molecular structure and charge transfer contributions to nonlinear optical property of 2-Methyl-4-nitroaniline: A DFT study

Journal of Molecular Structure, (1112): 63-70. 2016. 10.1016/j.molstruc.2016.02.013

Jeevitha, D.; Sadasivam, K.; Praveena, R.; Jayaprakasam, R.

DFT study of glycosyl group reactivity in quercetin derivatives

Journal of Molecular Structure, (1120): 15-24. 2016. 10.1016/j.molstruc.2016.05.003

Jenness, G. R.; Wan, W. M.; Chen, J. G. G.; Vlachos, D. G.

Reaction Pathways and Intermediates in Selective Ring Opening of Biomass-Derived Heterocyclic Compounds by Iridium

ACS Catalysis, (6): 7002-7009. 2016. 10.1021/acscatal.6b01310

Jerhaoui, S.; Chahdoura, F.; Rose, C.; Djukic, J. P.; Wencel-Delord, J.; Colobert, F.
Enantiopure Sulfinyl Aniline as a Removable and Recyclable Chiral Auxiliary for Asymmetric C(sp₃)-H Bond Activation
Chemistry-a European Journal, (22): 17397-17406. 2016. 10.1002/chem.201603507

Jesus, A. J. L.; Redinha, J. S.
Energetic and electronic study of indole derivatives
Structural Chemistry, (27): 809-820. 2016. 10.1007/s11224-015-0635-3

Ji, L. F.; Li, A. Y.; Li, Z. Z.; Ge, Z. X.
Substituent effects on the properties of the hemi-bonded complexes (XH₂P center dot center dot center dot NH₂Y)(+)
(X, Y=H, F, Cl, Br, NH₂, CH₃, OH)
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-015-2876-x

Jia, X. F.; Zhang, C. J.
Structure, bonding and reactivity of coinage metal complexes TML2 and TML2+ (TM = Cu, Ag, Au) with planar tetracoordinate carbon, a theoretical investigation
Computational and Theoretical Chemistry, (1075): 47-53. 2016. 10.1016/j.comptc.2015.11.010

Jia, X. F.; Zhang, C. J.
A Theoretical Investigation of the Rearrangement Reaction of Allylic Acetates Catalyzed by Au(I) Complexes with PtC
Acta Physico-Chimica Sinica, (32): 1434-1438. 2016. 10.3866/pku.Whxb201603101

Jia, Y. X.; Yang, X. Y.; Tay, W. S.; Li, Y. X.; Pullarkat, S. A.; Xu, K.; Hirao, H.; Leung, P. H.
Computational and carbon-13 NMR studies of Pt-C bonds in P-C-P pincer complexes
Dalton Transactions, (45): 2095-2101. 2016. 10.1039/c5dt02049b

Jian, J. W.; Jin, J. Y.; Qu, H.; Lin, H. L.; Chen, M. H.; Wang, G. J.; Zhou, M. F.; Andrada, D. M.; Hermann, M.; Frenking, G.
Observation of Main-Group Tricarbonyls B(CO)(3) and C(CO)(3) (+) Featuring a Tilted One-Electron Donor Carbonyl Ligand
Chemistry-a European Journal, (22): 2376-2385. 2016. 10.1002/chem.201504475

Jian, T.; Li, W. L.; Popov, I. A.; Lopez, G. V.; Chen, X.; Boldyrev, A. I.; Li, J.; Wang, L. S.
Manganese-centered tubular boron cluster-MnB16-: A new class of transition-metal molecules
Journal of Chemical Physics, (144) 2016. 10.1063/1.4946796

Jian, Z.; Yang, X. M.; Chen, D.; Qian, Y.
Theoretical studies of hydrogen bonding interactions between novolac resin and DMP-30
RSC Advances, (6): 114560-114565. 2016. 10.1039/c6ra24223e

Jiang, D. Y.; Sui, W.; Li, X. M.; Liu, B.; Wang, Q. W.; Pan, Y. R.
Synthesis, Crystal Structure and Theoretical Calculations of a Zinc(II) Coordination Polymer Assembled by Pyrazine-2,3-dicarboxylic Acid and Bis(imidazol) Ligands
Chinese Journal of Structural Chemistry, (35): 505-513. 2016.

Jiang, F.; Jin, T.; Zhu, X.; Tian, Z. Q.; Do-Thanh, C. L.; Hu, J.; Jiang, D. E.; Wang, H. L.; Liu, H. L.; Dai, S.
Substitution Effect Guided Synthesis of Task-Specific Nanoporous Polycarbazoles with Enhanced Carbon Capture
Macromolecules, (49): 5325-5330. 2016. 10.1021/acs.macromol.6b01342

Jiang, H.; Sun, Y. B.; Feng, J. W.; Wang, J.
Heterogeneous electro-Fenton oxidation of azo dye methyl orange catalyzed by magnetic Fe₃O₄ nanoparticles
Water Science and Technology, (74): 1116-1126. 2016. 10.2166/wst.2016.300

Jiang, J. X.; Liu, Y.; Hou, C.; Li, Y. W.; Luan, Z. H.; Zhao, C. Y.; Ke, Z. F.
Rationalization of the selectivity between 1,3-and 1,2-migration: a DFT study on gold(I)-catalyzed propargylic ester rearrangement
Organic & Biomolecular Chemistry, (14): 3558-3563. 2016. 10.1039/c6ob00215c

Jiang, Y. F.; Yang, L. J.; Wang, X. Z.; Wu, Q.; Ma, J.; Hu, Z.

Doping sp(2) carbon to boost the activity for oxygen reduction in an acidic medium: a theoretical exploration
RSC Advances, (6): 48498-48503. 2016. 10.1039/c6ra06473f

Jiang, Y. Y.; Yan, L.; Yu, H. Z.; Zhang, Q.; Fu, Y.
Mechanism of Vanadium-Catalyzed Selective C-O and C-C Cleavage of Lignin Model Compound
ACS Catalysis, (6): 4399-4410. 2016. 10.1021/acscatal.6b00239

Jiao, H. J.; Junge, K.; Alberico, E.; Beller, M.
A Comparative Computationally Study About the Defined M(II) Pincer Hydrogenation Catalysts (M = Fe, Ru, Os)
Journal of Computational Chemistry, (37): 168-176. 2016. 10.1002/jcc.23944

Jimenez-Izal, E.; Alexandrova, A. N.
sigma-Aromaticity in polyhydride complexes of Ru, Ir, Os, and Pt
Physical Chemistry Chemical Physics, (18): 11644-11652. 2016. 10.1039/c5cp04330a

Jin, B.; Jin, Q.; Jin, F. K.
Theoretical predictions on structures and p-, s-orbital aromaticities of the Hg₃B₃+/-3-, Hg₃B₃X (X = Li, Na, and K) and Hg₃B₃Mg+ clusters
Computational and Theoretical Chemistry, (1080): 66-71. 2016. 10.1016/j.comptc.2016.01.010

Jin, J.; Park, J. Y.; Lee, Y. S.
Optical Nature and Binding Energetics of Fluorescent Fluoride Sensor Bis(bora)calix 4 arene and Design Strategies of Its Homologues
Journal of Physical Chemistry C, (120): 24324-24334. 2016. 10.1021/acs.jpcc.6b06729

Jin, L. Q.; Melaimi, M.; Kostenko, A.; Karni, M.; Apeloig, Y.; Moore, C. E.; Rheingold, A. L.; Bertrand, G.
Isolation of cationic and neutral (allenylidene)(carbene) and bis(allenylidene)gold complexes
Chemical Science, (7): 150-154. 2016. 10.1039/c5sc03654b

Jin, P.; Liu, C.; Hou, Q. H.; Li, L. L.; Tang, C. C.; Chen, Z. F.
Scandium carbides/cyanides in the boron cage: computational prediction of X@B-80 (X = Sc₂C₂, Sc₃C₂, Sc₃CN and Sc₃C₂CN)
Physical Chemistry Chemical Physics, (18): 21398-21411. 2016. 10.1039/c6cp02884e

Jin, R.; Chen, X. H.; Du, Q.; Feng, H.; Xie, Y. M.; King, R. B.; Schaefer, H. F.
Binuclear iron carbonyl complexes of thialene
RSC Advances, (6): 82661-82668. 2016. 10.1039/c6ra14458f

Jin, R. Y.; Sun, X. H.; Liu, Y. F.; Long, W.; Chen, B.; Shen, S. Q.; Ma, H. X.
Synthesis, crystal structure, biological activity and theoretical calculations of novel isoxazole derivatives
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (152): 226-232. 2016.
10.1016/j.saa.2015.07.057

Jin, X. H.; Hu, B. C.
Crystal Structure and Properties of 7-Imino-3-Nitroimino-2,4,6,8-Tetraazabicyclo 3.3.0 Octane Hydrochloride
Zeitschrift fur Anorganische und Allgemeine Chemie, (642): 635-642. 2016. 10.1002/zaac.201600100

Jin, X. H.; Zhou, J. H.; Wang, S. J.; Hu, B. C.
COMPUTATIONAL STUDY ON STRUCTURE AND PROPERTIES OF NEW ENERGETIC MATERIAL 3,7-BIS(DINITROMETHYLENE)-2,4,6,8-TETRANITRO-2,4,6,8-TETRAAZA-BICYCLO 3. 3.0 OCTANE
Quimica Nova, (39): 467-473. 2016. 10.5935/0100-4042.20160054

Jin, X. L.; Qi, P. T.; Yang, H. H.; Zhang, Y.; Li, J. Y.; Chen, H. S.
Enhanced hydrogen adsorption on Li-coated B₁₂C₆N₆
Journal of Chemical Physics, (145) 2016. 10.1063/1.4964394

Jin, X. L.; Wu, S. P.; She, M. Y.; Jia, Y. F.; Hao, L. K.; Yin, B.; Wang, L. Y.; Obst, M.; Shen, Y. H.; Zhang, Y. M.; Li, J. L.

Novel Fluorescein-Based Fluorescent Probe for Detecting H₂S and Its Real Applications in Blood Plasma and Biological Imaging
Analytical Chemistry, (88): 11253-11260. 2016. 10.1021/acs.analchem.6b04087

Jitonnom, J.; Molloy, R.; Punyodom, W.; Meelua, W.
Theoretical studies on aluminum trialkoxide-initiated lactone ring opening polymerizations: Roles of alkoxide substituent and monomer ring structure
Computational and Theoretical Chemistry, (1097): 25-32. 2016. 10.1016/j.comptc.2016.10.009

Jorner, K.; Feixas, F.; Ayub, R.; Lindh, R.; Sola, M.; Ottosson, H.
Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic 10 Annulenyl Dicationic Rings
Chemistry-a European Journal, (22): 2793-2800. 2016. 10.1002/chem.201504924

Jotani, M. M.; Zukerman-Schpector, J.; Madureira, L. S.; Poplaukhin, P.; Arman, H. D.; Miller, T.; Tiekkink, E. R. T.
Structural, Hirshfeld surface and theoretical analysis of two conformational polymorphs of N,N'-bis(pyridin-3-ylmethyl)oxalamide
Zeitschrift Fur Kristallographie-Crystalline Materials, (231): 415-425. 2016. 10.1515/zkri-2016-1933

Joy, J.; Jose, A.; Jemmis, E. D.
Continuum in the X-Z-Y Weak Bonds: Z= Main Group Elements
Journal of Computational Chemistry, (37): 270-279. 2016. 10.1002/jcc.24036

Joy, M.; Alex, N.; Malayan, J. J.; Sudarsanakumar, C.; Mathews, A.
In Silico Quantum Chemical and Crystallographic Treatment of alpha-Formylketene Dithioacetal towards the Elucidation of Its Structural and Optical Nature
Chemistryselect, (1): 5974-5981. 2016. 10.1002/slct.201600988

Joy, S.; Sureshbabu, V. V.; Periyasamy, G.
Computational Studies on Structural, Excitation, and Charge-Transfer Properties of Ureidopeptidomimetics
Journal of Physical Chemistry B, (120): 6469-6478. 2016. 10.1021/acs.jpcb.6b02210

Juaristi, E.; Notario, R.
Theoretical Evidence for the Relevance of n(F) -> sigma(C-X) (X = H, C, O, S) Stereoelectronic Interactions*
Journal of Organic Chemistry, (81): 1192-1197. 2016. 10.1021/acs.joc.5b02718

Julia, F.; Garcia-Legaz, M. D.; Bautista, D.; Gonzalez-Herrero, P.
Influence of Ancillary Ligands and Isomerism on the Luminescence of Bis-cyclometalated Platinum(IV) Complexes
Inorganic Chemistry, (55): 7647-7660. 2016. 10.1021/acs.inorgchem.6b01100

Julia, F.; Gonzalez-Herrero, P.
Aromatic C-H Activation in the Triplet Excited State of Cyclometalated Platinum(II) Complexes Using Visible Light
Journal of the American Chemical Society, (138): 5276-5282. 2016. 10.1021/jacs.5b13311

Julia, F.; Gonzalez-Herrero, P.
Spotlight on the ligand: luminescent cyclometalated Pt(IV) complexes containing a fluorenyl moiety
Dalton Transactions, (45): 10599-10608. 2016. 10.1039/c6dt01722c

Jung, J. Y.; Kempe, D. K.; Yoon, S. H.; Gwini, N.; Fikes, A. G.; Marolf, D. M.; Parker, M. L.; Johnstone, J. E.; Powell, G. L.; Yang, L.; Nesterov, V. N.; Richmond, M. G.
Microwave-induced dppm ligand substitution in triosmium clusters: Structural and DFT evaluation of Os-3 clusters containing multiply activated dppm ligands through cyclometalation, ortho metalation, and P-C bond cleavage
Journal of Organometallic Chemistry, (813): 15-25. 2016. 10.1016/j.jorgchem.2016.03.018

Junior, R. V. A.; Moura, G. L. C.; Lima, N. B. D.
Insights into the spontaneity of hydrogen bond formation between formic acid and phthalimide derivatives
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3130-x

Kafentzi, M. C.; Orio, M.; Reglier, M.; Yao, S. L.; Kuhlmann, U.; Hildebrandt, P.; Driess, M.; Simaan, A. J.; Ray, K.

Changing the chemical and physical properties of high valent heterobimetallic bis-(mu-oxido) Cu-Ni complexes by ligand effects
Dalton Transactions, (45): 15994-16000. 2016. 10.1039/c6dt02391f

Kalita, B.
Tuning the Adsorption of Elemental Mercury by Small Gas-Phase Palladium Clusters: First-Principles Study
Journal of Physical Chemistry A, (120): 7714-7731. 2016. 10.1021/acs.jpca.6b06910

Kalpana, A.; Akilandeswari, L.
Expensive tripodal rotation in eta(6)-chromium tricarbonyl complexes of phosphabzenes-Insights from DFT study
Computational and Theoretical Chemistry, (1084): 103-108. 2016. 10.1016/j.comptc.2016.03.018

Kamalinahad, S.; Solimannejad, M.; Shakerzadeh, E.
Nonlinear Optical (NLO) Response of Pristine and Functionalized Dodecdehydrotribenzo 18 annulene (18 DBA): A Theoretical Study
Bulletin of the Chemical Society of Japan, (89): 692-699. 2016. 10.1246/bcsj.20160006

Kamalinahad, S.; Solimannejad, M.; Shakerzadeh, E.
Sensing of ozone (O-3) molecule via pristine singe-walled aluminum nitride nanotube: A DFT study
Superlattices and Microstructures, (89): 390-397. 2016. 10.1016/j.spmi.2015.11.032

Kanaani, A.; Ajloo, D.; Grivani, G.; Ghavami, A.; Vakili, M.
Tautomeric stability, molecular structure, NBO, electronic and NMR analyses of salicylideneimino-ethylimino-pentan-2-one
Journal of Molecular Structure, (1112): 87-96. 2016. 10.1016/j.molstruc.2016.02.024

Kanaani, A.; Ajloo, D.; Kiyani, H.; Ghasemian, H.; Vakili, M.; Feizabadi, M.
Molecular structure, spectroscopic investigations and computational study on the potential molecular switch of (E)-1-(4-(2-hydroxybenzylideneamino)phenyl)ethanone
Molecular Physics, (114): 2081-2097. 2016. 10.1080/00268976.2016.1178822

Kanazawa, Y.; Tsuji, H.; Ehara, M.; Fukuda, R.; Casher, D. L.; Tamao, K.; Nakatsuji, H.; Michl, J.
Electronic Transitions in Conformationally Controlled Peralkylated Hexasilanes
Chemphyschem, (17): 3010-3022. 2016. 10.1002/cphc.201600633

Kandemir, Z.; Mayda, S.; Bulut, N.
Electronic structure and correlations of vitamin B-12 studied within the Haldane-Anderson impurity model
European Physical Journal B, (89) 2016. 10.1140/epjb/e2016-60702-x

Kandhakumar, G.; Jothi, M.; Kumaradhas, P.
Probing the effect of nitro groups in nitramine based energetic molecules: a DFT and charge density study
Molecular Simulation, (42): 173-185. 2016. 10.1080/08927022.2015.1031130

Kang, G. J.; Song, C.; Ren, X. F.
Charge Transfer Enhancement in the D-pi-A Type Porphyrin Dyes: A Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT) Study
Molecules, (21) 2016. 10.3390/molecules21121618

Kang, J. J.; Zhang, X. X.; Zhou, H. J.; Gai, X. Q.; Jia, T.; Xu, L.; Zhang, J. J.; Li, Y. Q.; Ni, J.
1-D "Platinum Wire" Stacking Structure Built of Platinum(II) Diimine Bis(sigma-acetylide) Units with Luminescence in the NIR Region
Inorganic Chemistry, (55): 10208-10217. 2016. 10.1021/acs.inorgchem.6b01426

Kang, Y.; Tao, J.; Xue, Z. Y.; Zhang, Y.; Chen, Z. Q.; Xue, Y.
Quantum chemical exploration on the metabolic mechanisms of caffeine by flavin-containing monooxygenase
Tetrahedron, (72): 2858-2867. 2016. 10.1016/j.tet.2016.03.091

Kang, Y. K.; Park, H. S.

Propensities to form the beta-turn and beta-hairpin structures of D-Pro-Gly and Aib-D-Ala containing peptides: a computational study
New Journal of Chemistry, (40): 8565-8578. 2016. 10.1039/c6nj00614k

Kang, Y. K.; Yoo, I. K.
Propensities of Peptides Containing the Asn-Gly Segment to Form beta-Turn and beta-Hairpin Structures
Biopolymers, (105): 653-664. 2016. 10.1002/bip.22863

Karabacak, M.; Calisir, Z.; Kurt, M.; Kose, E.; Atac, A.
The spectroscopic (FT-IR, FT-Raman, dispersive Raman and NMR) study of ethyl-6-chloronicotinate molecule by combined density functional theory
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (153): 754-770. 2016.
10.1016/j.saa.2015.09.007

Karaush, N. N.; Bondarchuk, S. V.; Baryshnikov, G. V.; Minaeva, V. A.; Sun, W. H.; Minaev, B. F.
Computational study of the structure, UV-vis absorption spectra and conductivity of biphenylene-based polymers and their boron nitride analogues
RSC Advances, (6): 49505-49516. 2016. 10.1039/c6ra06832d

Karelson, M.; Dobchev, D. A.
QSAR of Heterocyclic Compounds in Large Descriptor Spaces
Heterocyclic Chemistry in the 21st Century: A Tribute to Alan Katritzky, Vol 120, (120): 237-273. 2016.
10.1016/bs.aihch.2016.03.006

Karhu, A. J.; Pakkanen, O. J.; Rautiainen, J. M.; Oilunkaniemi, R.; Chivers, T.; Laitinen, R. S.
The role of imidoselenium(II) chlorides in the formation of cyclic selenium imides via cyclocondensation
Dalton Transactions, (45): 6210-6221. 2016. 10.1039/c5dt04236d

Karimi, M.; Ignasiak, M. T.; Chan, B.; Croft, A. K.; Radom, L.; Schiesser, C. H.; Pattison, D. I.; Davies, M. J.
Reactivity of disulfide bonds is markedly affected by structure and environment: implications for protein modification and stability
Scientific Reports, (6) 2016. 10.1038/srep38572

Karir, G.; Fatima, M.; Viswanathan, K. S.
The elusive C-H center dot center dot center dot O complex in the hydrogen bonded systems of Phenylacetylene: A Matrix Isolation Infrared and Ab Initio Study
Journal of Chemical Sciences, (128): 1557-1569. 2016. 10.1007/s12039-016-1166-1

Karjalainen, M. M.; Sanchez-Perez, C.; Rautiainen, J. M.; Oilunkaniemi, R.; Laitinen, R. S.
Chalcogen-chalcogen secondary bonding interactions in trichalcogenaferrrocenophanes
Crystengcomm, (18): 4538-4545. 2016. 10.1039/c6ce00451b

Karri, R.; Banerjee, M.; Rai, R.; Roy, G.
*Synthesis and Characterization of 1:2 Complex of Mercury(II) Chloride with 1,3-Dimethyl-1*H*-Imidazole-2(3*H*)-Thione*
Proceedings of the National Academy of Sciences India Section a-Physical Sciences, (86): 611-617. 2016.
10.1007/s40010-016-0299-4

Kasende, O. E.; Nziko, V. D. N.; Scheiner, S.
H-bonding and stacking interactions between chloroquine and temozolomide
International Journal of Quantum Chemistry, (116): 1196-1204. 2016. 10.1002/qua.25152

Kasende, O. E.; Nziko, V. D. N.; Scheiner, S.
Interactions of Nucleic Acid Bases with Temozolomide. Stacked, Perpendicular, and Coplanar Heterodimers
Journal of Physical Chemistry B, (120): 9347-9361. 2016. 10.1021/acs.jpcb.6b06150

Kasende, O. E.; Nzuwah-Nziko, V. D.; Scheiner, S.
Interactions between temozolomide and quercetin
Structural Chemistry, (27): 1577-1588. 2016. 10.1007/s11224-016-0788-8

- Kathuria, D.; Arfeen, M.; Bankar, A. A.; Bharatam, P. V.
Carbene -> N+ Coordination Bonds in Drugs: A Quantum Chemical Study
Journal of Chemical Sciences, (128): 1607-1614. 2016. 10.1007/s12039-016-1173-2
- Katsamakas, S.; Papadopoulos, A. G.; Hadjipavlou-Litina, D.
Boronic Acid Group: A Cumbersome False Negative Case in the Process of Drug Design
Molecules, (21) 2016. 10.3390/molecules21091185
- Kaupp, M.; Karton, A.; Bischoff, F. A.
Al2O4 (-), a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods
Journal of Chemical Theory and Computation, (12): 3796-3806. 2016. 10.1021/acs.jctc.6b00594
- Kaur, D.; Kaur, R.; Shiekh, B. A.
Effects of substituents and charge on the RCHOa <-X-Y {X = Cl, Br, I; Y = -CF3, -CF2H, -CFH2, -CN, -CCH, -CCN; R = -OH, -OCH3, -NH2, -O-} halogen-bonded complexes
Structural Chemistry, (27): 961-971. 2016. 10.1007/s11224-015-0680-y
- Kaur, G.; Vikas
Global reaction route mapping of water-catalysed gas phase oxidation of glyoxylic acid with hydroxyl radical
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-2019-1
- Kaur, N.; Kumari, I.; Gupta, S.; Goel, N.
Spin Inversion Phenomenon and Two-State Reactivity Mechanism for Direct Benzene Hydroxylation by V4O10 Cluster
Journal of Physical Chemistry A, (120): 9588-9597. 2016. 10.1021/acs.jpca.6b08666
- Kaur, R.; Vikas
Exploring the role of a single water molecule in the tropospheric reaction of glycolaldehyde with an OH radical: a mechanistic and kinetics study
RSC Advances, (6): 29080-29098. 2016. 10.1039/c6ra01299j
- Kaviani, S.; Izadyar, M.; Housaindokht, M. R.
Solvent and spin state effects on molecular structure, IR spectra, binding energies and quantum chemical reactivity indices of deferiprone-ferric complex: DFT study
Polyhedron, (117): 623-627. 2016. 10.1016/j.poly.2016.06.041
- Kavitha, S.; Deepa, P.; Karthika, M.; Kanakaraju, R.
Topological analysis of metal-ligand and hydrogen bonds in transition metal hybrid structures - A computational study
Polyhedron, (115): 193-203. 2016. 10.1016/j.poly.2016.05.010
- Kavitha, T.; Velraj, G.
Structural, spectroscopic (FT-IR, FT-Raman, NMR) and computational analysis (DOS, NBO, Fukui) of 3,5-dimethylisoxazole and 4-(chloromethyl)-3,5-dimethylisoxazole: A DFT study
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500395
- Kaya, Y.
Density Functional Study of the Reaction Mechanism of Two Oxiimine Alcohol Formations and Their Novel Rearrangements
Helvetica Chimica Acta, (99): 333-346. 2016. 10.1002/hlca.201500155
- Kefalidis, C. E.; Jones, C.; Maron, L.
Mechanistic insights from theory on the reduction of CO₂, N₂O, and SO₂ molecules using tripodal diimine-enolate substituted magnesium(I) dimers
Dalton Transactions, (45): 14789-14800. 2016. 10.1039/c6dt02189a
- Kefalidis, C. E.; Maron, L.

Insights into the Cascade Reaction of CO and Heteroallenes Mediated by Dinitrogen Hafnocene Complexes: The Indirect Effect of Nitride's Nucleophilicity
Chemistry-a European Journal, (22): 4743-4747. 2016. 10.1002/chem.201600059

Kelley, M. P.; Yang, P.; Clark, S. B.; Clark, A. E.
Structural and Thermodynamic Properties of the Cm-III Ion Solvated by Water and Methanol
Inorganic Chemistry, (55): 4992-4999. 2016. 10.1021/acs.inorgchem.6b00477

Kelly, J. T.; McClellan, A. K.; Joe, L. V.; Wright, A. M.; Lloyd, L. T.; Tschumper, G. S.; Hammer, N. I.
Competition between Hydrophilic and Argyrophilic Interactions in Surface Enhanced Raman Spectroscopy
Chemphyschem, (17): 2782-2786. 2016. 10.1002/cphc.201600678

Kevorkyants, R.; Rudakova, A. V.; Chizhov, Y. V.; Bulanin, K. M.
The origin of 1560 cm(-1) band in experimental IR spectra of water adsorbed on TiO₂ surface: Ab initio assessment
Chemical Physics Letters, (662): 97-101. 2016. 10.1016/j.cplett.2016.09.014

Khadka, N.; Dean, D. R.; Smith, D.; Hoffman, B. M.; Raugei, S.; Seefeldt, L. C.
CO₂ Reduction Catalyzed by Nitrogenase: Pathways to Formate, Carbon Monoxide, and Methane
Inorganic Chemistry, (55): 8321-8330. 2016. 10.1021/acs.inorgchem.6b00388

Khalili, B.
A quantum chemical insight to intermolecular hydrogen bonding interaction between cytosine and nitrosamine: Structural and energetic investigations
Journal of Molecular Structure, (1107): 162-173. 2016. 10.1016/j.molstruc.2015.11.023

Khan, I.; Taha, M.; Pinho, S. P.; Coutinho, J. A. P.
Interactions of pyridinium, pyrrolidinium or piperidinium based ionic liquids with water: Measurements and COSMO-RS modelling
Fluid Phase Equilibria, (414): 93-100. 2016. 10.1016/j.fluid.2016.01.014

Khan, M. S.; Srivastava, A.
NH₃ and NO₂ adsorption analysis of GaN nanotube: A first principle investigation
Journal of Electroanalytical Chemistry, (775): 243-250. 2016. 10.1016/j.jelechem.2016.05.048

Khan, M. S.; Srivastava, A.; Pandey, R.
Electronic properties of a pristine and NH₃/NO₂ adsorbed buckled arsenene monolayer
RSC Advances, (6): 72634-72642. 2016. 10.1039/c6ra15005e

Kharnaior, K. S.; Devi, M.; Lyngdoh, R. H. D.
Generation of C₇H₇⁺ cations with isomerization reactions
Computational and Theoretical Chemistry, (1091): 150-164. 2016. 10.1016/j.comptc.2016.07.018

Khavani, M.; Izadyar, M.; Rezaeian, M.
A DFT study of solvent effects on the kinetics and mechanism of the 3,3 hetero-Cope rearrangement of 1-butene thiobenzoate
Progress in Reaction Kinetics and Mechanism, (41): 153-158. 2016. 10.3184/146867816x14634977847625

Kheirabadi, R.; Izadyar, M.
Computational Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic
Journal of Physical Chemistry A, (120): 10108-10115. 2016. 10.1021/acs.jpca.6b11437

Kheirabadi, R.; Izadyar, M.; Housiandokht, M. R.
Computational kinetic modeling of the selenol catalytic activity as the glutathione peroxidase nanomimic
Journal of Theoretical Biology, (409): 108-114. 2016. 10.1016/j.jtbi.2016.09.002

Khojastehnezhad, A.; Eshghi, H.; Moeinpour, F.; Bakavoli, M.; Izadyar, M.; Tajabadi, J.
Density functional theory study of the regio- and stereoselectivity of 1,3-dipolar cycloaddition reactions between 2-ethylthio-4-phenyl-1-azetin and some substituted nitrile oxides

Structural Chemistry, (27): 1041-1047. 2016. 10.1007/s11224-015-0703-8

Kidwell, N. M.; Mehta-Hurt, D. N.; Korn, J. A.; Zwier, T. S.

Infrared and Electronic Spectroscopy of the Jet-Cooled 5-Methyl-2-furanylmethyl Radical Derived from the Biofuel 2,5-Dimethylfuran

Journal of Physical Chemistry A, (120): 6434-6443. 2016. 10.1021/acs.jpca.6b05877

Kim, J.; Choi, J.; Kang, Y. S.; Won, J.

Matrix effect of mixed-matrix membrane containing CO₂-selective MOFs

Journal of Applied Polymer Science, (133) 2016. 10.1002/app.42853

Kinik, F. P.; Altintas, C.; Balci, V.; Koyuturk, B.; Uzun, A.; Keskin, S.

BMIM PF6 Incorporation Doubles CO₂ Selectivity of ZIF-8: Elucidation of Interactions and Their Consequences on Performance

ACS Applied Materials & Interfaces, (8): 30992-31005. 2016. 10.1021/acsami.6b11087

Kirshenboim, O.; Kozuch, S.

How to Twist, Split and Warp a sigma-Hole with Hypervalent Halogens

Journal of Physical Chemistry A, (120): 9431-9445. 2016. 10.1021/acs.jpca.6b07894

Klapotke, T. M.; Krumm, B.; Rest, S.; Scharf, R.; Schwabedissen, J.; Stammier, H. G.; Mitzel, N. W.

Carbonyl Diisocyanate CO(NCO)(2): Synthesis and Structures in Solid State and Gas Phase

Journal of Physical Chemistry A, (120): 4534-4541. 2016. 10.1021/acs.jpca.6b04245

Klein, M.; Schnakenburg, G.; Ferao, A. E.; Tokitoh, N.; Streubel, R.

Reactions of Li/Cl Phosphinidenoid Complexes with 1,3,4,5-Tetramethylimidazol-2-ylidene: A New Route to N-Heterocyclic Carbene Adducts of Terminal Phosphinidene Complexes and an Unprecedented Transformation of an Oxaphosphirane Complex

European Journal of Inorganic Chemistry: 685-690. 2016. 10.1002/ejic.201500959

Knezz, S. N.; Waltz, T. A.; Haenni, B. C.; Burrmann, N. J.; McMahon, R. J.

Spectroscopy and Photochemistry of Triplet 1,3-Dimethylpropynylidene (MeC₃Me)

Journal of the American Chemical Society, (138): 12596-12604. 2016. 10.1021/jacs.6b07444

Kobayashi, M.; Hayakawa, N.; Matsuo, T.; Li, B. L.; Fukunaga, T.; Hashizume, D.; Fueno, H.; Tanaka, K.; Tamao, K.

(Z)-1,2-Di(1-pyrenyl)disilene: Synthesis, Structure, and Intramolecular Charge-Transfer Emission

Journal of the American Chemical Society, (138): 758-761. 2016. 10.1021/jacs.5b11970

Kohler, M.; Koch, A.; Gorls, H.; Westerhausen, M.

Trimethylsilylmethylcalcium Iodide, an Easily Accessible Grignard-Type Reagent of a Heavy Alkaline Earth Metal

Organometallics, (35): 242-248. 2016. 10.1021/acs.organomet.5b00956

Kokhdan, S. N.; Reisi-Vanani, A.; Hamadanian, M.

Ab initio and TD-DFT study of the structural and spectroscopic properties of C₃₀H₁₀ as a new buckybowl

Fullerenes Nanotubes and Carbon Nanostructures, (24): 577-587. 2016. 10.1080/1536383x.2016.1207168

Kolar, M. H.; Hobza, P.

Computer Modeling of Halogen Bonds and Other sigma-Hole Interactions

Chemical Reviews, (116): 5155-5187. 2016. 10.1021/acs.chemrev.5b00560

Kolleth, A.; Lumbroso, A.; Tanriver, G.; Catak, S.; Sulzer-Mosse, S.; De Mesmaeker, A.

Synthesis of amino-cyclobutananes via 2+2 cycloadditions involving keteniminium intermediates

Tetrahedron Letters, (57): 2697-2702. 2016. 10.1016/j.tetlet.2016.04.092

Kolodziejczyk, W.; Kar, S.; Hill, G. A.; Leszczynski, J.

A comprehensive computational analysis of cathinone and its metabolites using quantum mechanical approaches and docking studies

Structural Chemistry, (27): 1291-1302. 2016. 10.1007/s11224-016-0779-9

- Komsa, D. N.; Staroverov, V. N.
Elimination of Spurious Fractional Charges in Dissociating Molecules by Correcting the Shape of Approximate Kohn-Sham Potentials
Journal of Chemical Theory and Computation, (12): 5361-5366. 2016. 10.1021/acs.jctc.6b00798
- Konarev, D. V.; Kuzmin, A. V.; Nakano, Y.; Faraonov, M. A.; Khasanov, S. S.; Otsuka, A.; Yamochi, H.; Saito, G.; Lyubovskaya, R. N.
Coordination Complexes of Transition Metals ($M = Mo, Fe, Rh, and Ru$) with Tin(II) Phthalocyanine in Neutral, Monoanionic, and Dianionic States
Inorganic Chemistry, (55): 1390-1402. 2016. 10.1021/acs.inorgchem.5b01906
- Konarev, D. V.; Kuzmin, A. V.; Nakano, Y.; Khasanov, S. S.; Ishikawa, M.; Otsuka, A.; Yamochi, H.; Saito, G.; Lyubovskaya, R. N.
SnPhPc phthalocyanines with dianion Pc^2- and radical trianion Pc center dot 3- macrocycles: syntheses, structures, and properties
Dalton Transactions, (45): 10780-10788. 2016. 10.1039/c6dt01132b
- Kondrashov, E. V.; Oznobikhina, L. P.; Aksamentova, T. N.; Chipanina, N. N.; Romanov, A. R.; Rulev, A. Y.
Basicity of the polydentate captodative aminoenones. Ab initio, DFT, and FTIR study
Journal of Physical Organic Chemistry, (29): 288-298. 2016. 10.1002/poc.3532
- Koparir, P.; Sarac, K.; Orek, C.; Koparir, M.
Molecular structure, spectroscopic properties and quantum chemical calculations of 8-t-butyl-4-methyl-2H-chromen-2-one
Journal of Molecular Structure, (1123): 407-415. 2016. 10.1016/j.molstruc.2016.07.046
- Kosai, T.; Ishida, S.; Iwamoto, T.
A Two-Coordinate Cyclic (Alkyl)(amino)silylene: Balancing Thermal Stability and Reactivity
Angewandte Chemie-International Edition, (55): 15554-15558. 2016. 10.1002/anie.201608736
- Koseki, J.; Gouda, H.; Hirono, S.
Molecular Orbital Study of the Formation of Intramolecular Hydrogen Bonding of a Ligand Molecule in a Protein Aromatic Hydrophobic Pocket
Chemical & Pharmaceutical Bulletin, (64): 1031-1035. 2016. 10.1248/cpb.c16-00126
- Kosnik, S. C.; Macdonald, C. L. B.
A zwitterionic triphosphonium compound as a tunable multifunctional donor
Dalton Transactions, (45): 6251-6258. 2016. 10.1039/c5dt03915k
- Kovacs, A.; Konings, R. J. M.
Molecular data of mixed metal oxides with importance in nuclear safety
Journal of Nuclear Materials, (477): 134-138. 2016. 10.1016/j.jnucmat.2016.05.015
- Koval, V. V.; Minyaev, R. M.; Minkin, V. I.
Geometric and Electronic Structures of Silicon Fluorides $SiFn(n=4)$ - ($N=4-6$) and Potential Energy Surfaces for Dissociation Reactions $SiF_5^- \rightarrow SiF_4 + F^-$ and $SiF_{62}^- \rightarrow SiF_5^- + F^-$
International Journal of Quantum Chemistry, (116): 1358-1361. 2016. 10.1002/qua.25184
- Kovrugin, V. M.; Gordon, E. E.; Kasapbasi, E. E.; Whangbo, M. H.; Colmont, M.; Siidra, O. I.; Colis, S.; Krivovichev, S. V.; Mentre, O.
Bonding Scheme, Hydride Character, and Magnetic Paths of $(HPO_3)^{2-}$ Versus $(SeO_3)^{2-}$ Building Units in Solids
Journal of Physical Chemistry C, (120): 1650-1656. 2016. 10.1021/acs.jpcc.5b10889
- Kozlova, S. G.; Adonin, S. A.; Sokolov, M. N.; Fedin, V. P.
Ability of lone electron pairs at Bi(III) and polymorphism of TBA(4) $Mo_8O_26(Bi_3)(2)$: Theoretical study
Inorganica Chimica Acta, (443): 1-6. 2016. 10.1016/j.ica.2015.12.020
- Kraka, E.; Setiawan, D.; Cremer, D.
Re-evaluation of the Bond Length-Bond Strength Rule: The Stronger Bond Is not Always the Shorter Bond

Journal of Computational Chemistry, (37): 130-142. 2016. 10.1002/jcc.24207

Krasnokutski, S. A.; Kuhn, M.; Kaiser, A.; Mauracher, A.; Renzler, M.; Bohme, D. K.; Scheier, P.

Building Carbon Bridges on and between Fullerenes in Helium Nanodroplets

Journal of Physical Chemistry Letters, (7): 1440-1445. 2016. 10.1021/acs.jpcllett.6b00462

Krasowska, M.; Bettinger, H. F.

Ring Enlargement of Three-Membered Boron Heterocycles upon Reaction with Organic Systems: Implications for the Trapping of Borylenes

Chemistry-a European Journal, (22): 10661-10670. 2016. 10.1002/chem.201600933

Krestyaninov, M. A.; Kiseleva, M. M.; Gomzina, N. A.; Kiseleva, M. G.

Conformational Manifold of Cryptand K 2.2.2. BB and Its Complex with Potassium Ion

Macroheterocycles, (9): 282-287. 2016. 10.6060/mhc160528k

Krewald, V.; Neese, F.; Pantazis, D. A.

Redox potential tuning by redox-inactive cations in nature's water oxidizing catalyst and synthetic analogues

Physical Chemistry Chemical Physics, (18): 10739-10750. 2016. 10.1039/c5cp07213a

Kubis, C.; Profir, I.; Fleischer, I.; Baumann, W.; Selent, D.; Fischer, C.; Spannenberg, A.; Ludwig, R.; Hess, D.; Franke, R.; Borner, A.

In Situ FTIR and NMR Spectroscopic Investigations on Ruthenium-Based Catalysts for Alkene Hydroformylation

Chemistry-a European Journal, (22): 2746-2757. 2016. 10.1002/chem.201504051

Kujawski, J.; Czaja, K.; Jodlowska, E.; Dettlaff, K.; Politanska, M.; Zwawiak, J.; Kujawski, R.; Ratajczak, T.; Chmielewski, M. K.; Bernard, M. K.

Structural and spectroscopic properties of econazole and sulconazole - Experimental and theoretical studies

Journal of Molecular Structure, (1119): 250-258. 2016. 10.1016/j.molstruc.2016.04.065

Kuklin, M. S.; Virkkunen, V.; Castro, P. M.; Izmer, V. V.; Kononovich, D. S.; Voskoboinikov, A. Z.; Linnolahti, M.

Quantitative structure-property relationships in propene polymerization by zirconocenes with a rac-SiMe₂ Ind (2) based ligand framework

Journal of Molecular Catalysis a-Chemical, (412): 39-46. 2016. 10.1016/j.molcata.2015.11.016

Kulish, K. I.; Novikov, A. S.; Tolstoy, P. M.; Bolotin, D. S.; Bokach, N. A.; Zolotarev, A. A.; Kukushkin, V. Y.

Solid state and dynamic solution structures of O-carbamidine amidoximes gives further insight into the mechanism of zinc(II)-mediated generation of 1,2,4-oxadiazoles

Journal of Molecular Structure, (1111): 142-150. 2016. 10.1016/j.molstruc.2016.01.038

Kumar, C. S. C.; Quah, C. K.; Balachandran, V.; Fun, H. K.; Asiri, A. M.; Chandraju, S.; Karabacak, M.

Synthesis, single crystal structure, spectroscopic characterization and molecular properties of (2E)-3-(2,6-dichlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one

Journal of Molecular Structure, (1116): 135-145. 2016. 10.1016/j.molstruc.2016.02.089

Kumar, J. S.; Devi, T. S. R.; Ramkumaar, G. R.; Bright, A.

Ab initio and density functional theory calculations of molecular structure and vibrational spectra of 4-(2-Hydroxyethyl) piperazine-1-ethanesulfonic acid

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (152): 509-522. 2016.

10.1016/j.saa.2015.07.084

Kumar, M.; Sinha, A.; Francisco, J. S.

Role of Double Hydrogen Atom Transfer Reactions in Atmospheric Chemistry

Accounts of Chemical Research, (49): 877-883. 2016. 10.1021/acs.accounts.6b00040

Kumar, N.; Seminario, J. M.

Lithium-Ion Model Behavior in an Ethylene Carbonate Electrolyte Using Molecular Dynamics

Journal of Physical Chemistry C, (120): 16322-16332. 2016. 10.1021/acs.jpcc.6b03709

Kumar, P.; Sengupta, A.; Deb, A. K. S.; Dasgupta, K.; Ali, S. M.

Sorption behaviour of Pu⁴⁺ and PuO₂²⁺ on amido amine-functionalized carbon nanotubes: experimental and computational study
RSC Advances, (6): 107011-107020. 2016. 10.1039/c6ra24184k

Kumar, R. S.; Almansour, A. I.; Arumugam, N.; Soliman, S. M.; Kumar, R. R.; Ghabbour, H. A.
Highly functionalized dispiro oxindole-pyrrolo 1,2-c thiazole-piperidone hybrid: Synthesis, characterization and theoretical investigations on the regiochemistry
Journal of Molecular Structure, (1121): 93-103. 2016. 10.1016/j.molstruc.2016.05.061

Kumar, V.; Sharma, J. N.; Achuthan, P. V.; Singh, D. K.; Ali, S. M.
A new bisglycolamide substituted calix 4 arene-benzo-crown-6 for the selective removal of cesium ion: combined experimental and density functional theoretical investigation
RSC Advances, (6): 47120-47129. 2016. 10.1039/c6ra05814k

Kumar, V. R.; Umapathy, S.
Solvent effects on the structure of the triplet excited state of xanthone: a time-resolved resonance Raman study
Journal of Raman Spectroscopy, (47): 1220-1230. 2016. 10.1002/jrs.4954

Kumar, V. R.; Verma, C.; Umapathy, S.
Molecular dynamics and simulations study on the vibrational and electronic solvatochromism of benzophenone
Journal of Chemical Physics, (144) 2016. 10.1063/1.4941058

Kumawat, J.; Gupta, V. K.; Vanka, K.
Effect of Donors on the Activation Mechanism in Ziegler-Natta Catalysis: A Computational Study
Chemcatchem, (8): 1809-1818. 2016. 10.1002/cctc.201600281

Kuriyama, S.; Arashiba, K.; Nakajima, K.; Matsuo, Y.; Tanaka, H.; Ishii, K.; Yoshizawa, K.; Nishibayashi, Y.
Catalytic transformation of dinitrogen into ammonia and hydrazine by iron-dinitrogen complexes bearing pincer ligand
Nature Communications, (7) 2016. 10.1038/ncomms12181

Kuroki, A.; Ushiyama, H.; Yamashita, K.
Theoretical studies on ammonia borane dehydrogenation catalyzed by iron pincer complexes
Computational and Theoretical Chemistry, (1090): 214-217. 2016. 10.1016/j.comptc.2016.06.017

Kurt, M.; Sas, E. B.; Can, M.; Okur, S.; Icli, S.; Demic, S.; Karabacak, M.; Jayavarthan, T.; Sundaraganesan, N.
Synthesis and spectroscopic characterization on 4-(2,5-di-2-thienyl-1H-pyrrol-1-yl) benzoic acid: A DFT approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (152): 8-17. 2016. 10.1016/j.saa.2015.07.058

Kus, N.
Theoretical and infrared investigation of 2-acetylpyridine isolated in solid nitrogen and in neat condensed phases
Journal of Molecular Structure, (1115): 214-219. 2016. 10.1016/j.molstruc.2016.02.076

Kusama, H.; Funaki, T.; Sayama, K.
A computational study on Ru complexes with bidentate carboxylate ligands: Insights into the photocurrents of dye-sensitized solar cells
Journal of Photochemistry and Photobiology a-Chemistry, (314): 171-177. 2016. 10.1016/j.jphotochem.2015.09.002

Kusama, H.; Sayama, K.
Comparative study on the interactions of TEMPO and iodine with organic dyes in dye-sensitized solar cells
Journal of Photochemistry and Photobiology a-Chemistry, (330): 95-101. 2016. 10.1016/j.jphotochem.2016.07.030

Kusevska, E.; Montero-Campillo, M. M.; Mo, O.; Yanez, M.
Boron-Boron One-Electron Sigma Bonds versus B-X-B Bridged Structures
Chemistry-a European Journal, (22): 13697-13704. 2016. 10.1002/chem.201600976

Kutudila, P.; Linguerri, R.; Al-Mogren, M. M.; Pichon, C.; Condon, S.; Hochlaf, M.
First principle investigations of organobismuth palladium-catalyzed C-C coupling reaction: mechanism, chemoselectivity and solvent effects

Kuznetsov, A. E.

Computational design of ZnP(P)(4) stacks: Three modes of binding

Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500437

Kuznetsov, A. E.

How the change of the ligand from L = porphine, P2-, to L = P-4-substituted porphine, P(P)(4)(2-), affects the electronic properties and the M-L binding energies for the first-row transition metals M = Sc-Zn: Comparative study

Chemical Physics, (469): 38-48. 2016. 10.1016/j.chemphys.2016.02.010

Kyri, A. W.; Majhi, P. K.; Sasamori, T.; Agou, T.; Nesterov, V.; Guo, J. D.; Nagase, S.; Tokitoh, N.; Streubel, R.

Synthesis of a 1-Aryl-2,2-chlorosilyl(phospha)silene Coordinated by an N-Heterocyclic Carbene

Molecules, (21) 2016. 10.3390/molecules21101309

Lachowicz, J. I.; Nurchi, V. M.; Crisponi, G.; Jaraquemada-Pelaez, M. G.; Arca, M.; Pintus, A.; Santos, M. A.; Quintanova, C.; Gano, L.; Szewczuk, Z.; Zoroddu, M. A.; Peana, M.; Dominguez-Martin, A.; Choquesillo-Lazarte, D.

Hydroxypyridinones with enhanced iron chelating properties. Synthesis, characterization and in vivo tests of 5-hydroxy-2-(hydroxymethyl) pyridine-4(1H)-one

Dalton Transactions, (45): 6517-6528. 2016. 10.1039/c6dt00129g

Lagodzinskaya, G. V.; Laptinskaya, T. V.; Kazakov, A. I.; Kurochkina, L. S.; Manelis, G. B.

Slow large-scale supramolecular structuring as a cause of kinetic anomalies in the liquid-phase oxidation with nitric acid

Russian Chemical Bulletin, (65): 984-992. 2016. 10.1007/s11172-016-1401-4

Lambic, N. S.; Sommer, R. D.; Ison, E. A.

Transition-Metal Oxos as the Lewis Basic Component of Frustrated Lewis Pairs

Journal of the American Chemical Society, (138): 4832-4842. 2016. 10.1021/jacs.6b00705

Lamsabhi, A.; Vallejos, M. M.; Herrera, B.; Mo, O.; Yanez, M.

Effect of beryllium bonds on the keto-enol tautomerism of formamide derivatives: a subtle basicity-acidity balance

Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1902-0

Landis, C. R.; Weinhold, F.

18-Electron Rule and the 3c/4e Hyperbonding Saturation Limit

Journal of Computational Chemistry, (37): 237-241. 2016. 10.1002/jcc.24001

Langer, J.; Kosygin, I.; Puchta, R.; Pahl, J.; Harder, S.

A Soft Grip: Magnesium Complexes with a Phosphine-Modified Phosphonium Diylidic Lewis Base

Chemistry-a European Journal, (22): 17425-17435. 2016. 10.1002/chem.201603775

Lannes, A.; Manceau, A.; Rovezzi, M.; Glatzel, P.; Joly, Y.; Gautier-Luneau, I.

Intramolecular Hg center dot center dot center dot pi interactions of d-character with non-bridging atoms in mercury-aryl complexes

Dalton Transactions, (45): 14035-14038. 2016. 10.1039/c6dt02200f

Lao, K. U.; Herbert, J. M.

Energy Decomposition Analysis with a Stable Charge-Transfer Term for Interpreting Intermolecular Interactions

Journal of Chemical Theory and Computation, (12): 2569-2582. 2016. 10.1021/acs.jctc.6b00155

Lao, K. U.; Liu, K. Y.; Richard, R. M.; Herbert, J. M.

Understanding the many-body expansion for large systems. II. Accuracy considerations

Journal of Chemical Physics, (144) 2016. 10.1063/1.4947087

Lashley, M. A.; Ivanov, A. S.; Bryantsev, V. S.; Dai, S.; Hancock, R. D.

Highly Preorganized Ligand 1,10-Phenanthroline-2,9-dicarboxylic Acid for the Selective Recovery of Uranium from Seawater in the Presence of Competing Vanadium Species

Inorganic Chemistry, (55): 10818-10829. 2016. 10.1021/acs.inorgchem.6b02234

Latrous, L.; Salpin, J. Y.; Haldys, V.; Leon, E.; Correia, C.; Lamsabhi, A.

Gas-phase interactions of organotin compounds with cysteine

Journal of Mass Spectrometry, (51): 1006-1015. 2016. 10.1002/jms.3812

Laurella, S. L.; Erben, M. F.

Comment on "Structural and vibrational studies on 1-(5-Methyl- 1,3,4 thiadiazol-2-yl)-pyrrolidin-2-ol" Spectrochimica Acta Part A, 152 (2016) 252-261 . The importance of intramolecular OH center dot center dot center dot N hydrogen bonding in the conformational properties of thiadiazol-pyrrolidin-2-ol bearing species
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (164): 40-42. 2016. 10.1016/j.saa.2016.03.018

Ledet, A. D.; Hudnall, T. W.

Reduction of a diamidocarbene-supported borenium cation: isolation of a neutral boryl-substituted radical and a carbene-stabilized aminoborylene
Dalton Transactions, (45): 9820-9826. 2016. 10.1039/c6dt00300a

Lee, J. H.; Woo, J. G.; Shong, B.

Tunable adsorption of isocyanides on group 14 (100)-2 x 1 surfaces

Applied Surface Science, (390): 968-973. 2016. 10.1016/j.apsusc.2016.09.013

Lee, S. J. R.; Mullinax, J. W.; Schaefer, H. F.

Intermolecular interactions and proton transfer in the hydrogen halide-superoxide anion complexes
Physical Chemistry Chemical Physics, (18): 6201-6208. 2016. 10.1039/c5cp05878c

Lee, V. Y.; Gapurenko, O. A.; Ito, Y.; Meguro, T.; Sugawara, H.; Sekiguchi, A.; Minyaev, R. M.; Minkin, V. I.; Herber, R. H.; Gornitzka, H.

Pyramidananes: The Covalent Form of the Ionic Compounds

Organometallics, (35): 346-356. 2016. 10.1021/acs.organomet.5b00924

Lee, V. Y.; Sugawara, H.; Gapurenko, O. A.; Minyaev, R. M.; Minkin, V. I.; Gornitzka, H.; Sekiguchi, A.

A Cationic Phosphapyramidane

Chemistry-a European Journal, (22): 17585-17589. 2016. 10.1002/chem.201604480

Leem, G.; Morseth, Z. A.; Wee, K. R.; Jiang, J. L.; Brennaman, M. K.; Papanikolas, J. M.; Schanze, K. S.

Polymer-Based Ruthenium(II) Polypyridyl Chromophores on TiO₂ for Solar Energy Conversion

Chemistry-an Asian Journal, (11): 1257-1267. 2016. 10.1002/asia.201501384

Leenaraj, D. R.; Manimaran, D.; Joe, I. H.

Molecular docking and structural analysis of non-opioid analgesic drug acetaminophen with halogen substitution: A DFT approach

Journal of Molecular Structure, (1123): 180-190. 2016. 10.1016/j.molstruc.2016.06.035

Lefkidis, G.; Reyes, S. A.

Quasianalytical treatment of the spin Seebeck effect on the Na-2 molecule

Physical Review B, (94) 2016. 10.1103/PhysRevB.94.144433

Leoncini, A.; Mohapatra, P. K.; Bhattacharyya, A.; Raut, D. R.; Sengupta, A.; Verma, P. K.; Tiwari, N.; Bhattacharyya, D.; Jha, S.; Wouda, A. M.; Huskens, J.; Verboom, W.

Unique selectivity reversal in Am³⁺-Eu³⁺ extraction in a tripodal TREN-based diglycolamide in ionic liquid: extraction, luminescence, complexation and structural studies

Dalton Transactions, (45): 2476-2484. 2016. 10.1039/c5dt04729c

Lepetit, C.; Maraval, V.; Canac, Y.; Chauvin, R.

On the nature of the dative bond: Coordination to metals and beyond. The carbon case

Coordination Chemistry Reviews, (308): 59-75. 2016. 10.1016/j.ccr.2015.07.018

Levine, D. S.; Horn, P. R.; Mao, Y. Z.; Head-Gordon, M.

Variational Energy Decomposition Analysis of Chemical Bonding. 1. Spin-Pure Analysis of Single Bonds
Journal of Chemical Theory and Computation, (12): 4812-4820. 2016. 10.1021/acs.jctc.6b00571

Levitskaya, A. I.; Kalinin, A. A.; Fominykh, O. D.; Vasilyev, I. V.; Balakina, M. Y.

Nonlinear optical properties of chromophores with indolizine donors: Theoretical study
Computational and Theoretical Chemistry, (1094): 17-22. 2016. 10.1016/j.comptc.2016.08.021

Lewis, A. K.; Dunleavy, K. M.; Senkow, T. L.; Her, C.; Horn, B. T.; Jerset, M. A.; Mahling, R.; McCarthy, M. R.; Perell, G. T.; Valley, C. C.; Karim, C. B.; Gao, J. L.; Pomerantz, W. C. K.; Thomas, D. D.; Cembran, A.; Hinderliter, A.; Sachs, J. N.

Oxidation increases the strength of the methionine-aromatic interaction
Nature Chemical Biology, (12): 860-. 2016. 10.1038/nchembio.2159

Li, C. Z.; Li, D. L.; Ma, C.; Liu, Y. F.

DFT-TDDFT investigation of excited-state intramolecular proton transfer in 2-(2'-hydroxyphenyl)benzimidazole derivatives: Effects of electron acceptor and donor groups
Journal of Molecular Liquids, (224): 83-88. 2016. 10.1016/j.molliq.2016.09.088

Li, D. Z.; Li, R.; Zhang, L. J.; Ou, T.; Zhai, H. J.

Planar B3S2H3- and B3S2H3 clusters with a five-membered B3S2 ring: boron-sulfur hydride analogues of cyclopentadiene
Physical Chemistry Chemical Physics, (18): 21412-21420. 2016. 10.1039/c6cp03952a

Li, H.; Wu, C.; Malinin, S. V.; Tretiak, S.; Chernyak, V. Y.

Exciton scattering approach for optical spectra calculations in branched conjugated macromolecules
Chemical Physics, (481): 124-132. 2016. 10.1016/j.chemphys.2016.08.033

Li, H. D.; Feng, H.; Xie, Y. M.; Schaefer, H. F.

The Recently Synthesized Dimagnesiabutadiene and the Analogous Dimetalla-Beryllium, -Calcium, -Strontium, and -Barium Compounds
Chemistry-a European Journal, (22): 15019-15026. 2016. 10.1002/chem.201603355

Li, J.; Liu, S.; Lu, X. H.

Theoretical Study of the Mechanism for Direct Addition of Hydride to CO₂ on Ruthenium Complexes: Nature of Ru-H Bond and Effect of Hydrogen Bonding
Bulletin of the Chemical Society of Japan, (89): 905-910. 2016. 10.1246/bcsj.20160084

Li, J. B.; Ramos, G. D.; Rogachev, A. Y.

Stability of functionalized corannulene cations R-C₂₀H₁₀ (+): An influence of the nature of R-Group
Journal of Computational Chemistry, (37): 2266-2278. 2016. 10.1002/jcc.24444

Li, J. B.; Rogachev, A. Y.

Aromatic stabilization of functionalized corannulene cations
Physical Chemistry Chemical Physics, (18): 11781-11791. 2016. 10.1039/c5cp07002c

Li, J. J.; Li, J. H.; Zhang, D. J.; Liu, C. B.

DFT Study on the Mechanism of Formic Acid Decomposition by a Well-Defined Bifunctional Cyclometalated Iridium(III) Catalyst: Self-Assisted Concerted Dehydrogenation via Long-Range Intermolecular Hydrogen Migration
ACS Catalysis, (6): 4746-4754. 2016. 10.1021/acscatal.6b00564

Li, J. L.; Zhou, S. D.; Zhang, J.; Schlangen, M.; Usharani, D.; Shaik, S.; Schwarz, H.

Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions
Journal of the American Chemical Society, (138): 11368-11377. 2016. 10.1021/jacs.6b07246

Li, J. L.; Zhou, S. D.; Zhang, J.; Schlangen, M.; Weiske, T.; Usharani, D.; Shaik, S.; Schwarz, H.

Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations XYO₂ (+) (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer
Journal of the American Chemical Society, (138): 7973-7981. 2016. 10.1021/jacs.6b03798

- Li, K. X.; Yan, Y. B.; Zhao, J.; Lei, J. X.; Jia, X. L.; Mushrif, S. H.; Yang, Y. H.
Understanding the role of hydrogen bonding in Bronsted acidic ionic liquid-catalyzed transesterification: a combined theoretical and experimental investigation
Physical Chemistry Chemical Physics, (18): 32723-32734. 2016. 10.1039/c6cp06502c
- Li, L.; Huang, C. Y.; Jiang, X. N.; Gao, X. C.; Wang, C. S.
Ionic Hydrogen Bonding Between Arginine Side Chain and Nucleic Acid Bases
Chemical Journal of Chinese Universities-Chinese, (37): 1460-1467. 2016. 10.7503/cjcu20160346
- Li, L.; Zhang, Y.; Chang, Z. M.; Bai, F. Q.; Zhang, H. X.; Ferri, J. K.; Dong, W. F.
Theoretical study on fluorescent probes for cyanide based on the indolium functional group
Organic Electronics, (30): 1-11. 2016. 10.1016/j.orgel.2015.12.002
- Li, L. C.; Wang, W.; Wang, X. L.; Zhang, L.
Investigating the mechanism of the selective hydrogenation reaction of cinnamaldehyde catalyzed by Pt-n clusters
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3039-4
- Li, L. C.; Wei, W.; Wang, W.; Wang, X. L.; Zhang, L.; Tian, A. M.
Selective hydrogenation of cinnamaldehyde catalyzed by Co-doped Pt clusters: a density functional theoretical study
RSC Advances, (6): 88277-88286. 2016. 10.1039/c6ra16150b
- Li, L. C.; Zhang, L.; Wang, W.; Pan, R.; Mao, S.; Tian, A. M.
Investigation on the Mechanism for C-N Coupling of 3-Iodopyridine and Pyrazole Catalyzed by Cu(I)
International Journal of Chemical Kinetics, (48): 11-22. 2016. 10.1002/kin.20966
- Li, M. R.; Wang, G. C.
Computational study on gold-catalyzed (4+3) intramolecular cycloaddition of trienyne: mechanism, reactivity and selectivity
RSC Advances, (6): 73454-73468. 2016. 10.1039/c6ra17436a
- Li, P.; Li, Y.; Chen, C.; Wang, L.; Zhang, J. L.
Catalytic performance of a series of guanidinium-based ionic liquids in the coupling reaction of carbon dioxide with epoxides
RSC Advances, (6): 87036-87043. 2016. 10.1039/c6ra20174a
- Li, Q. Z.; Zheng, J. J.; He, L.; Nagase, S.; Zhao, X.
Stabilization of a Chlorinated C-#4348(66)-C-2v Cage by Encapsulating Monometal Species: Coordination between Metal and Double Hexagon-Condensed Pentalenes
Inorganic Chemistry, (55): 7667-7675. 2016. 10.1021/acs.inorgchem.6b01134
- Li, R. Z.; Hou, G. L.; Liu, C. W.; Xu, H. G.; Zhao, X.; Gao, Y. Q.; Zheng, W. J.
Initial hydration behavior of sodium iodide dimer: photoelectron spectroscopy and ab initio calculations
Physical Chemistry Chemical Physics, (18): 557-565. 2016. 10.1039/c5cp05550d
- Li, S.; Wang, Y. C.; Wang, X. L.; Zhang, Y. W.
Theoretical investigation on activation of ethene by the HNbN- anion in the gas phase
Computational and Theoretical Chemistry, (1096): 74-79. 2016. 10.1016/j.comptc.2016.10.003
- Li, S. B.; Tang, C. M.; Zhang, X.
How will the benzyne group -C6H4 affect the structure, electronic and optical properties of M3N@C-80 (M = Sc, Y)?
Computational and Theoretical Chemistry, (1084): 17-24. 2016. 10.1016/j.comptc.2016.03.019
- Li, S. Y.; Wu, D.; Li, Y.; Yu, D.; Liu, J. Y.; Li, Z. R.
Insight into structural and pi-magnesium bonding characteristics of the X2Mg center dot center dot center dot Y (X = H, F; Y = C2H2, C2H4 and C6H6) complexes
RSC Advances, (6): 102754-102761. 2016. 10.1039/c6ra23368f

- Li, W.; Li, Y. Z.; Lin, R. C.; Li, S. H.
Generalized Energy-Based Fragmentation Approach for Localized Excited States of Large Systems
Journal of Physical Chemistry A, (120): 9667-9677. 2016. 10.1021/acs.jpca.6b11193
- Li, W.; Zeng, Y. L.; Li, X. Y.; Sun, Z.; Meng, L. P.
Insight into the pseudo pi-hole interactions in the M3H6 center dot center dot center dot center dot(NCF)(n) (M = C, Si, Ge, Sn, Pb; n=1, 2, 3) complexes
Physical Chemistry Chemical Physics, (18): 24672-24680. 2016. 10.1039/c6cp03713e
- Li, W. L.; Liu, H. T.; Jian, T.; Lopez, G. V.; Piazza, Z. A.; Huang, D. L.; Chen, T. T.; Su, J.; Yang, P.; Chen, X.; Wang, L. S.; Li, J.
Bond-bending isomerism of Au2I3: competition between covalent bonding and aurophilicity
Chemical Science, (7): 475-481. 2016. 10.1039/c5sc03568f
- Li, W. Y.; Huang, D. F.; Lyu, Y. J.
A comparative computational study of N-heterocyclic olefin and N-heterocyclic carbene mediated carboxylative cyclization of propargyl alcohols with CO2
Organic & Biomolecular Chemistry, (14): 10875-10885. 2016. 10.1039/c6ob01901c
- Li, W. Y.; Yang, N.; Lyu, Y. J.
Theoretical Insights into the Catalytic Mechanism of N-Heterocyclic Olefins in Carboxylative Cyclization of Propargyl Alcohol with CO2
Journal of Organic Chemistry, (81): 5303-5313. 2016. 10.1021/acs.joc.6b00559
- Li, X. J.; Claes, P.; Haertelt, M.; Lievens, P.; Janssens, E.; Fielicke, A.
Structural determination of niobium-doped silicon clusters by far-infrared spectroscopy and theory
Physical Chemistry Chemical Physics, (18): 6291-6300. 2016. 10.1039/c5cp07298k
- Li, X. J.; Yan, Z. J.; Li, S. N.
The nature of structure and bonding between transition metal and mixed Si-Ge tetramers: A 20-electron superatom system
Journal of Computational Chemistry, (37): 2316-2323. 2016. 10.1002/jcc.24456
- Li, X. M.; Sun, M.; Pan, Y. R.; Ji, J. Y.
Synthesis, Crystal Structure and Theoretical Calculations of a New Co(II) Coordination Polymer Based on 5-Nitroisophthalic Acid and Bis(imidazol) Ligands
Chinese Journal of Structural Chemistry, (35): 298-306. 2016.
- Li, X. M.; Wang, Q. W.; Zhan, P. Y.; Pan, Y. R.
Synthesis, Crystal Structure and Theoretical Calculations of a Cadmium(II) Coordination Polymer Assembled by 4,4'-Oxydibenzoic Acid and 1,3-Bis(imidazol-1-ylmethyl)Benzene Ligands
Journal of Chemical Crystallography, (46): 163-169. 2016. 10.1007/s10870-016-0641-3
- Li, X. Y.
Electron density properties and metallophilic interactions of coinage metal halides M2X2 (M = Cu, Ag and Au, X = F-I): Ab initio calculation
Materials Research Express, (3) 2016. 10.1088/2053-1591/3/11/115702
- Li, X. Y.; Cai, J. X.
Electron Density Properties and Metallophilic Interactions of Gold Halides AuX2 and Au2X (X = F-I): Ab Initio Calculations
International Journal of Quantum Chemistry, (116): 1350-1357. 2016. 10.1002/qua.25183
- Li, Y.; Du, S. W.
Understanding the mechanisms, regioselectivities and enantioselectivities of the DMAP-catalyzed 2+4 cycloaddition of gamma-methyl allenolate and phenyl(phenyldiazenyl)methanone
RSC Advances, (6): 84177-84186. 2016. 10.1039/c6ra16321a
- Li, Y.; Du, S. W.; Du, Z.; Chen, C. M.

A theoretical study of DABCO and PPh₃ catalyzed annulations of allenoates with azodicarboxylate
RSC Advances, (6): 82260-82269. 2016. 10.1039/c6ra19308k

Li, Y. J.; Chan, P. K.; Leong, W. K.

C-C reductive coupling mediated by attack at a spectator ligand

Journal of Organometallic Chemistry, (810): 40-45. 2016. 10.1016/j.jorganchem.2016.03.004

Li, Y. J.; Chen, J. W.; Qiao, X. L.; Zhang, H. M.; Zhang, Y. N.; Zhou, C. Z.

Insights into photolytic mechanism of sulfapyridine induced by triplet-excited dissolved organic matter

Chemosphere, (147): 305-310. 2016. 10.1016/j.chemosphere.2015.12.115

Li, Y. J.; Ganguly, R.; Leong, W. K.

*An Arbusov-type reaction with the bis(alkynyl) iridium complex Cp*Ir(L)(C₂Ar)(2)*

Journal of Organometallic Chemistry, (818): 42-47. 2016. 10.1016/j.jorganchem.2016.05.018

Li, Y. J.; Leong, W. K.

*Intramolecular Cycloaddition in the (Diyne) iridium Complexes Cp*Ir(CO)(eta(2)-ArC CC CAr) : An Experimental and Computational Study*

European Journal of Inorganic Chemistry: 4769-4773. 2016. 10.1002/ejic.201600579

Li, Y. J.; Tam, N. M.; Woodham, A. P.; Lyon, J. T.; Li, Z.; Lievens, P.; Fielicke, A.; Nguyen, M. T.; Janssens, E.

Structure Dependent Magnetic Coupling in Cobalt-Doped Silicon Clusters

Journal of Physical Chemistry C, (120): 19454-19460. 2016. 10.1021/acs.jpcc.6b06320

Li, Y. K.; Yuan, Z.; Zhao, Y. X.; Zhao, C. Y.; Liu, Q. Y.; Chen, H.; He, S. G.

Thermal Methane Conversion to Syngas Mediated by Rh-1-Doped Aluminum Oxide Cluster Cations RhAl₃O₄+

Journal of the American Chemical Society, (138): 12854-12860. 2016. 10.1021/jacs.6b05454

Li, Y. P.; Head-Gordon, M.; Bell, A. T.

Theoretical Study of 4-(Hydroxymethyl)benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)furoic Acid

Catalyzed by Sn-BEA

ACS Catalysis, (6): 5052-5061. 2016. 10.1021/acscatal.6b01160

Li, Y. W.; Hou, C.; Jiang, J. X.; Zhang, Z. H.; Zhao, C. Y.; Page, A. J.; Ke, Z. F.

General H-2 Activation Modes for Lewis Acid-Transition Metal Bifunctional Catalysts

ACS Catalysis, (6): 1655-1662. 2016. 10.1021/acscatal.5b02395

Li, Z. S.; Chen, X. D.; Li, Y. Q.; Su, C. Y.; Grutzmacher, H.

N-Heterocyclic carbene phosphaketene adducts as precursors to carbene-phosphinidene adducts and a rearranged pi-system

Chemical Communications, (52): 11343-11346. 2016. 10.1039/c6cc05916c

Liang, H. S.; Bi, S. W.; Liu, Y. X.; Tang, Y. N.; Liu, C. C.

Theoretical study on Au(I)-catalyzed 2+2+2 cycloadditions of ynamides with two discrete nitriles

Organic & Biomolecular Chemistry, (14): 2637-2644. 2016. 10.1039/c5ob02568k

Liang, J. X.; Su, Q.; Zhao, D. Z.; Wang, Y. B.; Li, G. H.; Geng, Z. Y.

Comparative Computational Study of Hydrogen Abstraction Reactions of CY₃H + XO⁻ (X = F, Cl, and Br)

Heteroatom Chemistry, (27): 199-209. 2016. 10.1002/hc.21317

Lightcap, J.; Hester, T. H.; Kamena, K.; Albury, R. M.; Pruitt, C. J. M.; Goebbert, D. J.

Gas-Phase Fragmentation of Aluminum Oxide Nitrate Anions Driven by Reactive Oxygen Radical Ligands

Journal of Physical Chemistry A, (120): 1501-1507. 2016. 10.1021/acs.jpca.5b12417

Lightcap, J.; Hester, T. H.; Patterson, D.; Butler, J. T.; Goebbert, D. J.

Formation of a Spin-Forbidden Product, (1) MnO₄ (-), from Gas-Phase Decomposition of (6) Mn(NO₃)₃ (-)

Journal of Physical Chemistry A, (120): 7071-7079. 2016. 10.1021/acs.jpca.6b06978

- Limas, N. G.; Manz, T. A.
Introducing DDEC6 atomic population analysis: part 2. Computed results for a wide range of periodic and nonperiodic materials
RSC Advances, (6): 45727-45747. 2016. 10.1039/c6ra05507a
- Lin, B. B.; Ma, G. C.; Liu, Y. J.
Mechanism of the Glutathione Persulfide Oxidation Process Catalyzed by Ethylmalonic Encephalopathy Protein 1
ACS Catalysis, (6): 7010-7020. 2016. 10.1021/acscatal.6b01417
- Lin, B. B.; Su, H.; Ma, G. C.; Liu, Y. J.; Hou, Q. Q.
Theoretical study of the hydrolysis mechanism of dihydrocoumarin catalyzed by serum paraoxonase 1 (PON1): different roles of Glu53 and His115 for catalysis
RSC Advances, (6): 60376-60384. 2016. 10.1039/c6ra09735a
- Lin, C. Z.; Liu, Q.; Zhang, Y.; Liu, J.; Zheng, C. G.
DFT investigation of the ring contraction reaction of (eta(4)-1,2-disilacyclohexadiene)iron tricarbonyls: a crucial intramolecular Si-Si bond activation
Organic Chemistry Frontiers, (3): 480-485. 2016. 10.1039/c5qo00402k
- Lin, X. F.; Chen, B. L.; Xi, Y. Y.; Wang, C. Y.; Fu, H.
The substituent effect of the pentafluorophenyl groups on ruthenium-porphyrin-catalyzed intramolecular amidation of sulfamate ester: A DFT study
Computational and Theoretical Chemistry, (1080): 1-9. 2016. 10.1016/j.comptc.2016.01.020
- Liu, B. G.; Zeng, J.; Chen, C.; Liu, Y. L.; Ma, H. J.; Mo, H. Z.; Liang, G. Z.
Interaction of cinnamic acid derivatives with beta-cyclodextrin in water: Experimental and molecular modeling studies
Food Chemistry, (194): 1156-1163. 2016. 10.1016/j.foodchem.2015.09.001
- Liu, G. R.; Zhan, J. Y.; Zhao, Y. Y.; Li, L.; Jiang, X. X.; Fu, J. J.; Li, C. P.; Zheng, M. H.
Distributions, profiles and formation mechanisms of polychlorinated naphthalenes in cement kilns co-processing municipal waste incinerator fly ash
Chemosphere, (155): 348-357. 2016. 10.1016/j.chemosphere.2016.04.069
- Liu, J.; Herbert, J. M.
Pair-Pair Approximation to the Generalized Many-Body Expansion: An Alternative to the Four-Body Expansion for ab Initio Prediction of Protein Energetics via Molecular Fragmentation
Journal of Chemical Theory and Computation, (12): 572-584. 2016. 10.1021/acs.jctc.5b00955
- Liu, J. B.; Sheng, X. H.; Sun, C. Z.; Huang, F.; Chen, D. Z.
A Computational Mechanistic Study of Amidation of Quinoline N-Oxide: The Relative Stability of Amido Insertion Intermediates Determines the Regioselectivity
ACS Catalysis, (6): 2452-2461. 2016. 10.1021/acscatal.5b02938
- Liu, J. H.; Zheng, Y. Y.; Liu, Y.; Yuan, H. Y.; Zhang, J. P.
Mechanistic Insight on (E)-Methyl 3-(2-Aminophenyl)Acrylate Cyclization Reaction by Multicatalysis of Solvent and Substrate
Journal of Computational Chemistry, (37): 2386-2394. 2016. 10.1002/jcc.24463
- Liu, K.; Kang, Y.; Ma, G. H.; Mohwald, H.; Yan, X. H.
Molecular and mesoscale mechanism for hierarchical self-assembly of dipeptide and porphyrin light-harvesting system
Physical Chemistry Chemical Physics, (18): 16738-16747. 2016. 10.1039/c6cp01358a
- Liu, L.; Osorio, E.; Heine, T.
Understanding the Central Location of a Hexagonal Hole in a B-36 Cluster
Chemistry-an Asian Journal, (11): 3220-3224. 2016. 10.1002/asia.201601106
- Liu, L.; Vankova, N.; Heine, T.
A kinetic study on the reduction of CO₂ by frustrated Lewis pairs: from understanding to rational design

Physical Chemistry Chemical Physics, (18): 3567-3574. 2016. 10.1039/c5cp06925d

Liu, L.; Wei, J. N.; Chi, Y.; Zhang, W. X.; Xi, Z. F.

Structure and Reaction Chemistry of Magnesium Organocuprates Derived from Magnesiacyclopentadienes and Copper(I) Salts

Angewandte Chemie-International Edition, (55): 14762-14765. 2016. 10.1002/anie.201607355

Liu, L.; Wu, Y. L.; Chen, P.; Chan, C. L.; Xu, J.; Zhu, J.; Zhao, Y. F.

Mechanism, catalysis and predictions of 1,3,2-diazaphospholenes: theoretical insight into highly polarized P-X bonds
Organic Chemistry Frontiers, (3): 423-433. 2016. 10.1039/c6qo00002a

Liu, M.; Nieger, M.; Hubner, E. G.; Schmidt, A.

Formation of N-Heterocyclic Carbenes by Tautomerization of Mesomeric Betaines: Cyclic Boron Adducts and Palladium Complexes From 2-(Imidazolium-1-yl)phenolates

Chemistry-a European Journal, (22): 5416-5424. 2016. 10.1002/chem.201505042

Liu, M. C.; Chen, H. F.; Huang, W. J.; Chin, C. H.; Chen, S. C.; Huang, T. P.; Wu, Y. J.

Photochemistry and infrared spectrum of single-bridged diborane(5) anion isolated in solid argon
Journal of Chemical Physics, (145) 2016. 10.1063/1.4961262

Liu, M. S.; Gao, K. Q.; Liang, L.; Sun, J. M.; Sheng, L.; Arai, M.

Experimental and theoretical insights into binary Zn-SBA-15/KI catalysts for the selective coupling of CO₂ and epoxides into cyclic carbonates under mild conditions

Catalysis Science & Technology, (6): 6406-6416. 2016. 10.1039/c6cy00725b

Liu, M. X.; Li, Q. Z.; Cheng, J. B.; Li, W. Z.; Li, H. B.

Tetrel bond of pseudohalide anions with XH₃F (X = C, Si, Ge, and Sn) and its role in S(N)2 reaction
Journal of Chemical Physics, (145) 2016. 10.1063/1.4971855

Liu, M. X.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.

Tetrel bonds between PySiX₃ and some nitrogenated bases: Hybridization, substitution, and cooperativity
Journal of Molecular Graphics & Modelling, (65): 35-42. 2016. 10.1016/j.jmgm.2016.02.005

Liu, M. X.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.; McDowell, S. A. C.

Comparison of hydrogen, halogen, and tetrel bonds in the complexes of HArF with YH₃X (X = halogen, Y = C and Si)
RSC Advances, (6): 19136-19143. 2016. 10.1039/c5ra23556a

Liu, M. X.; Yang, L.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.; Xiao, B.; Yu, X. F.

Modulating the strength of tetrel bonding through beryllium bonding
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3060-7

Liu, M. X.; Zhuo, H. Y.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.

Theoretical study of the cooperative effects between the triel bond and the pnicogen bond in BF₃ center dot center dot center dot NCXH₂ center dot center dot center dot center dot Y (X = P, As, Sb; Y = H₂O, NH₃) complexes
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-015-2882-z

Liu, Q.; Li, Z. S.; Chen, S. L.

Metal -Embedded Graphene as Potential Counter Electrode for Dye-Sensitized Solar Cell
Industrial & Engineering Chemistry Research, (55): 455-462. 2016. 10.1021/acsiecr.5b03464

Liu, Q. Z.; Qiu, L.; Wang, Y.; Lv, G. C.; Liu, G. Q.; Wang, S. S.; Lin, J. G.

Solvent effect on molecular structure, IR spectra, thermodynamic properties and chemical stability of zoledronic acid: DFT study
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2953-9

Liu, R. R.; Lu, Y. H.; Geng, Z. Y.; Yan, P. J.

Study of mechanism of cyclohexane dehydrogenation by gas-phase Ti-2(+) cationic dimer in mixed PESs
Computational and Theoretical Chemistry, (1090): 203-213. 2016. 10.1016/j.comptc.2016.06.022

- Liu, S. B.
Information-Theoretic Approach in Density Functional Reactivity Theory
Acta Physico-Chimica Sinica, (32): 98-118. 2016. 10.3866/pku.Whxb201510302
- Liu, W. D.; Cheng, L. J.
Size Evolution of the 2e-Superatom in Ligand-Protected Au Nanoclusters: Au-2-(AuL)(1-12) (L = Cl, SH, SCH3, PH2, and P(CH3)(2))
Journal of Physical Chemistry C, (120): 2432-2438. 2016. 10.1021/acs.jpcc.5b10612
- Liu, X. S.; Lei, D.; Gan, L. H.
Structures and Properties of Endohedral Metallofullerene Sc2S@C-86
Acta Physico-Chimica Sinica, (32): 929-934. 2016. 10.3866/pku.Whxb201601221
- Liu, Y.; Luo, Z. J.; Zhang, J. Z.; Xia, F.
DFT Calculations on the Mechanism of Transition-Metal-Catalyzed Reaction of Diazo Compounds with Phenols: O-H Insertion versus C-H Insertion
Journal of Physical Chemistry A, (120): 6485-6492. 2016. 10.1021/acs.jpca.6b05735
- Liu, Y.; Ojamae, L.
C-13 Chemical Shift in Natural Gas Hydrates from First-Principles Solid-State NMR Calculations
Journal of Physical Chemistry C, (120): 1130-1136. 2016. 10.1021/acs.jpcc.5b11372
- Liu, Y.; Tian, Z. M.; Cheng, L. J.
Size evolution and ligand effects on the structures and stability of (AuL)(n) (L = Cl, SH, SCH3, PH2, P(CH3)(2), n=1-13) clusters
RSC Advances, (6): 4705-4712. 2016. 10.1039/c5ra22741k
- Liu, Y.; Yu, Z. Z.; Luo, Z. J.; Zhang, J. Z.; Liu, L.; Xia, F.
Mechanistic Investigation of Aromatic C(sp²)-H and Alkyl C(sp³)-H Bond Insertion by Gold Carbenes
Journal of Physical Chemistry A, (120): 1925-1932. 2016. 10.1021/acs.jpca.6b00636
- Liu, Y. M.; Liu, Y. D.; Zhong, R. G.; Peng, B.; Schaefer, H. F.
Effects of heavy metal ions on N-nitrosodimethylamine (NDMA) formation
RSC Advances, (6): 70474-70479. 2016. 10.1039/c6ra11481d
- Liu, Y. M.; Wang, X.; Liu, Y. D.; Zhong, R. G.; Xie, Y. M.; Schaefer, H. F.
1,1-Dilithioethylene: Toward Spectroscopic Identification of the Definitive Singlet Ground Electronic State of a Peculiar Structure
Chemphyschem, (17): 1623-1629. 2016. 10.1002/cphc.201600051
- Liu, Y. Y.; Ren, S. J.; Huang, J.; Liang, Y. T.; Wei, X. G.; Ren, Y.; Lau, K. C.; Zhu, J.
Comprehensive Comparison Between the Gas-phase S(N)2 Reactions at Carbon and at Nitrogen
Current Organic Chemistry, (20): 1058-1068. 2016. 10.2174/1385272820666151026231003
- Liu, Z. L.; Zou, J. H.; Qin, Z. B.; Xie, H.; Fan, H. J.; Tang, Z. C.
Photoelectron Velocity Map Imaging Spectroscopy of Lead Tetracarbonyl-Iron Anion PbFe(CO)(4)(-)
Journal of Physical Chemistry A, (120): 3533-3538. 2016. 10.1021/acs.jpca.6b02786
- Liu, Z. M.; Pottel, J.; Shahamat, M.; Tomberg, A.; Labute, P.; Moitessier, N.
Elucidating Hyperconjugation from Electronegativity to Predict Drug Conformational Energy in a High Throughput Manner
Journal of Chemical Information and Modeling, (56): 788-801. 2016. 10.1021/acs.jcim.6b00012
- Lizardo-Huerta, J. C.; Sirjean, B.; Bounaceur, R.; Fournet, R.
Intramolecular effects on the kinetics of unimolecular reactions of beta-HOROO center dot and HOQ(center dot)OOH radicals
Physical Chemistry Chemical Physics, (18): 12231-12251. 2016. 10.1039/c6cp00111d

- Lopez, C. S.; Faza, O. N.; De Proft, F.; Kocolouris, A.
Assessing the Attractive/Repulsive Force Balance in Axial Cyclohexane C-H-ax center dot center dot center dot Y-ax Contacts: A Combined Computational Analysis in Monosubstituted Cyclohexanes
Journal of Computational Chemistry, (37): 2647-2658. 2016. 10.1002/jcc.24496
- Lopez, C. S.; Faza, O. N.; Freindorf, M.; Kraka, E.; Cremer, D.
Solving the Pericyclic Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives
Journal of Organic Chemistry, (81): 404-414. 2016. 10.1021/acs.joc.5b01997
- Lopez, R. V.; Faza, O. N.; Lopez, C. S.
Conformational control allows for 3,3 -sigmatropic rearrangements to proceed with torquoselectivity
RSC Advances, (6): 59181-59184. 2016. 10.1039/c6ra10789c
- Louie, M. K.; Francisco, J. S.; Verdicchio, M.; Klippenstein, S. J.; Sinha, A.
Dimethylamine Addition to Formaldehyde Catalyzed by a Single Water Molecule: A Facile Route for Atmospheric Carbinolamine Formation and Potential Promoter of Aerosol Growth
Journal of Physical Chemistry A, (120): 1358-1368. 2016. 10.1021/acs.jpca.5b04887
- Lu, B.; Zhang, X. Y.; Meng, L. P.; Zeng, Y. L.
The Pt (II)center dot center dot Cl Interactions: Nature and Strength
Chemistryselect, (1): 5698-5705. 2016. 10.1002/slct.201601230
- Lu, J. S.; Su, S. H.; Yang, M. C.; Wen, X. T.; Xie, J. Z.; Su, M. D.
Substituent Effects on Boron-Bismuth Triple Bond: A New Target for Synthesis
Organometallics, (35): 3924-3931. 2016. 10.1021/acs.organomet.6b00659
- Lu, N.; Bu, Y. X.; Wang, H. T.
Intensified effects of multi-Cu modification on the electronic properties of the modified base pairs containing hetero-ring-expanded pyrimidine bases
Physical Chemistry Chemical Physics, (18): 2913-2923. 2016. 10.1039/c5cp06133d
- Lu, N. M.; Chung, W. C.; Ley, R. M.; Lin, K. Y.; Francisco, J. S.; Negishi, E.
Molecularly Tuning the Radicaloid N-H center dot center dot center dot O = C Hydrogen Bond
Journal of Physical Chemistry A, (120): 1307-1315. 2016. 10.1021/acs.jpca.6b00144
- Lu, R. Q.; Liu, D.; Lu, Y. K.; Wang, S. T.
The nature of interactions between Cu₂Cl₃ (-)-based ionic liquid and thiophene - A theoretical study
Journal of Saudi Chemical Society, (20): 303-306. 2016. 10.1016/j.jscs.2013.04.002
- Lu, S. J.; Xu, X. L.; Feng, G.; Xu, H. G.; Zheng, W. J.
Structural and Electronic Properties of AuSin- (n=4-12) Clusters: Photoelectron Spectroscopy and Ab Initio Calculations
Journal of Physical Chemistry C, (120): 25628-25637. 2016. 10.1021/acs.jpcc.6b08598
- Lui, M. W.; Paisley, N. R.; McDonald, R.; Ferguson, M. J.; Rivard, E.
Metal-Free Dehydrogenation of Amine-Boranes by Tunable N-Heterocyclic Iminoboranes
Chemistry-a European Journal, (22): 2134-2145. 2016. 10.1002/chem.201503528
- Lummis, J. A. M.; Perras, F. A.; McDonald, R.; Bryce, D. L.; Fogg, D. E.
Sterically Driven Olefin Metathesis: The Impact of Alkylidene Substitution on Catalyst Activity
Organometallics, (35): 691-698. 2016. 10.1021/acs.organomet.5b00984
- Luo, J.; Wang, C. Z.; Lan, J. H.; Wu, Q. Y.; Zhao, Y. L.; Chai, Z. F.; Nie, C. M.; Shi, W. Q.
Theoretical studies on the complexation of Eu(III) and Am(III) with HDEHP: structure, bonding nature and stability
Science China-Chemistry, (59): 324-331. 2016. 10.1007/s11426-015-5489-4
- Luo, M.; Zhu, C. Q.; Chen, L. N.; Zhang, H.; Xia, H. P.
Halogenation of carbyne complexes: isolation of unsaturated metallaiodirenium ion and metallabromirenium ion

Chemical Science, (7): 1815-1818. 2016. 10.1039/c5sc03963k

Lutters, D.; Merk, A.; Schmidtmann, M.; Muller, T.

The Silicon Version of Phosphine Chalcogenides: Synthesis and Bonding Analysis of Stabilized Heavy Silaaldehydes
Inorganic Chemistry, (55): 9026-9032. 2016. 10.1021/acs.inorgchem.6b01510

Ma, F.; Miao, T.; Zhou, Z. J.; Xu, H. L.

Excess-electron-induced C-C bond formation in transformation of carbon dioxide
RSC Advances, (6): 851-858. 2016. 10.1039/c5ra17187c

Ma, F.; Miao, T.; Zhou, Z. J.; Xu, H. L.

A theoretical study on CO₂ inserting into C-H bond
Chemical Physics Letters, (647): 46-50. 2016. 10.1016/j.cplett.2016.01.034

Ma, G. L.; Li, Z. H.

Methane activation by metal-free Lewis acid centers only - a computational design and mechanism study
Physical Chemistry Chemical Physics, (18): 11539-11549. 2016. 10.1039/c6cp00505e

Ma, H. M.; Wang, J.; Zhao, H. Y.; Zhang, D. B.; Liu, Y.

Structural prediction for scandium carbide monolayer sheet
Chemical Physics Letters, (660): 238-243. 2016. 10.1016/j.cplett.2016.08.034

Ma, J. F.; Ma, F.; Zhou, Z. J.; Liu, Y. T.

Theoretical investigation of boron-doped lithium clusters, BLin (n=3-6), activating CO₂: an example of the carboxylation of C-H bonds
RSC Advances, (6): 84042-84049. 2016. 10.1039/c6ra15152c

Ma, P. P.; Wang, Y. C.; Wang, W. X.; Deng, Z. P.; Niu, G. P.; Wang, X. L.; Li, S.; Zhang, Y. W.

Theoretical investigation on activation of C-H and C-C bonds of 2-butyne by gas-phase Nb atom
Computational and Theoretical Chemistry, (1085): 23-30. 2016. 10.1016/j.comptc.2016.03.033

Mabkhout, Y. N.; Aldawsari, F. D.; Al>Showiman, S. S.; Barakat, A.; Soliman, S. M.; Choudhary, M. I.; Yousuf, S.; Ben Hadda, T.; Mubarak, M. S.

Synthesis, Molecular Structure Optimization, and Cytotoxicity Assay of a Novel 2-Acetyl-3-amino-5-(2-oxopropyl)sulfanyl-4-cyanothiophene
Molecules, (21) 2016. 10.3390/molecules21020214

Macdonald, C. L. B.; Binder, J. F.; Swidan, A.; Nguyen, J. H.; Kosnik, S. C.; Ellis, B. D.

Convenient Preparation and Detailed Analysis of a Series of NHC-Stabilized Phosphorus(I) Dyes and Their Derivatives
Inorganic Chemistry, (55): 7152-7166. 2016. 10.1021/acs.inorgchem.6b01163

Macetti, G.; Loconte, L.; Rizzato, S.; Gatti, C.; Lo Presti, L.

Intermolecular Recognition of the Antimalarial Drug Chloroquine: A Quantum Theory of Atoms in Molecules-Density Functional Theory Investigation of the Hydrated Dihydrogen Phosphate Salt from the 103 K X-ray Structure
Crystal Growth & Design, (16): 6043-6054. 2016. 10.1021/acs.cgd.6b01069

Machado, C. M. B.; Santos, V. F. C.; Belarmino, M.; Franca, J. A. A.; Moura, G. L. C.; Lima, N. B. D.

Effect of 1,10-phenanthroline aromaticity in carboxylic acids: H-1 NMR spectroscopy, GIAO calculations and thermodynamic properties
Journal of Molecular Structure, (1118): 279-287. 2016. 10.1016/j.molstruc.2016.04.031

MacInnis, M. C.; DeMott, J. C.; Zolnhofer, E. M.; Zhou, J.; Meyer, K.; Hughes, R. P.; Ozerov, O. V.

Cationic Two-Coordinate Complexes of Pd(I) and Pt(I) Have Longer Metal-Ligand Bonds Than Their Neutral Counterparts
Chem, (1): 902-920. 2016. 10.1016/j.chempr.2016.11.007

Maeda, C.; Shimonishi, J.; Miyazaki, R.; Hasegawa, J.; Ema, T.

Highly Active and Robust Metalloporphyrin Catalysts for the Synthesis of Cyclic Carbonates from a Broad Range of Epoxides and Carbon Dioxide
Chemistry-a European Journal, (22): 6556-6563. 2016. 10.1002/chem.201600164

Mafune, F.; Kudoh, S.; Takenouchi, M.
Role of Gold Atoms in Oxidation and Reduction of Cationic Rhodium-Gold Oxide Clusters, RhnAumOk+, Studied by Thermal Desorption Spectrometry and DFT Calculations
Journal of Physical Chemistry C, (120): 19280-19285. 2016. 10.1021/acs.jpcc.6b06982

Mafune, F.; Takenouchi, M.; Miyajima, K.; Kudoh, S.
Rhodium Oxide Cluster Ions Studied by Thermal Desorption Spectrometry
Journal of Physical Chemistry A, (120): 356-363. 2016. 10.1021/acs.jpca.5b09531

Magnuson, K. W.; Oshiro, S. M.; Gurr, J. R.; Yoshida, W. Y.; Gernbicky, M.; Rheingold, A. L.; Hughes, R. P.; Cain, M. F.
Streamlined Preparation and Coordination Chemistry of Hybrid Phosphine-Phosphaalkene Ligands
Organometallics, (35): 855-859. 2016. 10.1021/acs.organomet.6b00101

Magubane, M. N.; Nyamato, G. S.; Ojwach, S. O.; Munro, O. Q.
Structural, kinetic, and DFT studies of the transfer hydrogenation of ketones mediated by (pyrazole)pyridine iron(II) and nickel(II) complexes
RSC Advances, (6): 65205-65221. 2016. 10.1039/c6ra12788f

Maheeswari, R.; Manjula, J.
"Vibrational spectroscopic analysis and molecular docking studies of (E)-4-methoxy-N'-(4-methylbenzylidene)benzohydrazide by DFT"
Journal of Molecular Structure, (1115): 144-155. 2016. 10.1016/j.molstruc.2016.02.066

Mahi, M. A.; Mekelleche, S. M.; Benchouk, W.; Aurell, M. J.; Domingo, L. R.
Theoretical study of the regio- and stereoselectivity of the intramolecular Povarov reactions yielding 5H-chromeno 2,3-c acridine derivatives
RSC Advances, (6): 15759-15769. 2016. 10.1039/c5ra25184b

Mahmoudi, G.; Afkhami, F. A.; Jena, H. S.; Nematollahi, P.; Esrafili, M. D.; Garczarek, P.; Van Hecke, K.; Gargari, M. S.; Kirillov, A. M.
Halide ion-driven self-assembly of Zn(ii) compounds derived from an asymmetrical hydrazone building block: a combined experimental and theoretical study
New Journal of Chemistry, (40): 10116-10126. 2016. 10.1039/c6nj01534d

Mahmoudi, G.; Bauza, A.; Frontera, A.
Concurrent agostic and tetrel bonding interactions in lead(II) complexes with an isonicotinohydrazide based ligand and several anions
Dalton Transactions, (45): 4965-4969. 2016. 10.1039/c6dt00131a

Mahmoudi, G.; Bauza, A.; Rodriguez-Dieguez, A.; Garczarek, P.; Kaminsky, W.; Frontera, A.
Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis studies of carbohydrazone based on Zn(II) complexes
CrystEngComm, (18): 102-112. 2016. 10.1039/c5ce01915j

Mahmoudi, S.; Jamalizadeh, E.; Hosseini, S. M. A.
Corrosion of iron and aluminum in acidic and basic media: theoretical and experimental investigation
Anti-Corrosion Methods and Materials, (63): 329-336. 2016. 10.1108/acmm-09-2014-1439

Mai, B. K.; Kim, Y.
Is It Fe(III)-Oxyl Radical That Abstracts Hydrogen in the C-H Activation of TauD? A Theoretical Study Based on the DFT Potential Energy Surfaces
Inorganic Chemistry, (55): 3844-3852. 2016. 10.1021/acs.inorgchem.5b02939

Maihom, T.; Choomwattana, S.; Wannakao, S.; Probst, M.; Limtrakul, J.

Ethylene Epoxidation with Nitrous Oxide over Fe-BTC Metal-Organic Frameworks: A DFT Study
Chemphyschem, (17): 3416-3422. 2016. 10.1002/cphc.201600836

Maiores, L.; Aragoni, M. C.; Carcangiu, G.; Cocco, O.; Isaia, F.; Lippolis, V.; Meloni, P.; Murru, A.; Slawin, A. M. Z.; Tuveri, E.; Woollins, J. D.; Arca, M.

Oxamate salts as novel agents for the restoration of marble and limestone substrates: case study of ammonium N-phenyloxamate

New Journal of Chemistry, (40): 2768-2774. 2016. 10.1039/c5nj02505b

Majerz, I.

Proton Transfer Influence on Geometry and Electron Density in Benzoic Acid-Pyridine Complexes
Helvetica Chimica Acta, (99): 286-295. 2016. 10.1002/hlca.201500183

Majumdar, S.; Maiti, S.; Dastidar, S. G.

Dynamic and Static Water Molecules Complement the TN16 Conformational Heterogeneity inside the Tubulin Cavity
Biochemistry, (55): 335-347. 2016. 10.1021/acs.biochem.5b00853

Makarewicz, E.; Gordon, A. J.; Berski, S.

The electronic structure of the xenon insertion compounds XXe-MX₂ (X = F, Cl, Br, I; M = B, Al, Ga)
Polyhedron, (117): 97-109. 2016. 10.1016/j.poly.2016.05.025

Makiabadi, B.; Zakarianezhad, M.; Masoodi, H. R.; Bagheri, S.; Noormandi, F.

Theoretical study of physicochemical properties of ionic liquid mim C(CN)(3)

Chemistry of Heterocyclic Compounds, (52): 244-252. 2016. 10.1007/s10593-016-1875-x

Makkos, E.; Kerridge, A.; Austin, J.; Kaltsoyannis, N.

Ionic adsorption on the brucite (0001) surface: A periodic electrostatic embedded cluster method study
Journal of Chemical Physics, (145) 2016. 10.1063/1.4968035

Maldonado-Dominguez, M.; Ruiz-Perez, K.; Gonzalez-Antonio, O.; Romero-Avila, M.; Mendez-Stivalet, J.; Flores-Perez, B.

On the Brassard's rule of regioselectivity in Diels-Alder reactions between haloquinones and polar dienes
RSC Advances, (6): 75194-75201. 2016. 10.1039/c6ra14073d

Malinowski, P. J.; Himmel, D.; Krossing, I.

Silver Complexes of Dihalogen Molecules

Angewandte Chemie-International Edition, (55): 9259-9261. 2016. 10.1002/anie.201603741

Manceau, A.; Enescu, M.; Simionovici, A.; Lanson, M.; Gonzalez-Rey, M.; Rovezzi, M.; Tucoulou, R.; Glatzel, P.; Nagy, K. L.; Bourdineaud, J. P.

Chemical Forms of Mercury in Human Hair Reveal Sources of Exposure

Environmental Science & Technology, (50): 10721-10729. 2016. 10.1021/acs.est.6b03468

Mandal, S.; Nandi, S.; Anoop, A.; Chattaraj, P. K.

Viability of aromatic all-pnictogen anions

Physical Chemistry Chemical Physics, (18): 11738-11745. 2016. 10.1039/c5cp07236k

Mansour, A. M.

Influence of metal complex formation on the antimicrobial activity of nifuroxazide: spectroscopic, electrochemical, and DFT studies

Journal of Coordination Chemistry, (69): 215-226. 2016. 10.1080/00958972.2015.1111344

Mansour, A. M.

Spectroscopic, DFT, magnetic and biological activity evaluation of Pd(II), Pt(II) and Ru(III) complexes of Nitazoxanide
Inorganica Chimica Acta, (453): 697-703. 2016. 10.1016/j.ica.2016.09.031

Mansour, A. M.

Tazarotene copper complexes: Synthesis, crystal structure, DFT and biological activity evaluation

Polyhedron, (109): 99-106. 2016. 10.1016/j.poly.2016.01.041

- Mansour, A. M.
Thermal, spectral, DFT and biological activity evaluation of Co(II), Ni(II) and Cu(II) complexes of N,S-chelated benzotriazole ligand
Journal of Thermal Analysis and Calorimetry, (123): 571-581. 2016. 10.1007/s10973-015-4978-1
- Mansour, A. M.; El Bakry, E. M.; Abdel-Ghani, N. T.
Co(II), Ni(II) and Cu(II) complexes of methyl-5-(Phenylthio) benzimidazole-2-carbamate: Molecular structures, spectral and DFT calculations
Journal of Molecular Structure, (1111): 100-107. 2016. 10.1016/j.molstruc.2016.01.060
- Mansour, A. M.; El Bakry, E. M.; Abdel-Ghani, N. T.
Flubendazole Pd(II) complexes: structural studies, cytotoxicity, and quantum chemical calculations
Journal of the Iranian Chemical Society, (13): 1429-1437. 2016. 10.1007/s13738-016-0858-2
- Mansour, A. M.; El Bakry, E. M.; Abdel-Ghani, N. T.
Photocatalytic degradation of methylene blue with copper(II) oxide synthesized by thermal decomposition of Flubendazole complexes
Journal of Photochemistry and Photobiology a-Chemistry, (327): 21-24. 2016. 10.1016/j.jphotochem.2016.04.022
- Mansour, A. M.; Shehab, O. R.
Experimental and quantum chemical calculations of novel photoactivatable manganese(I) tricarbonyl complexes
Journal of Organometallic Chemistry, (822): 91-99. 2016. 10.1016/j.jorgchem.2016.08.018
- Manz, T. A.; Limas, N. G.
Introducing DDEC6 atomic population analysis: part 1. Charge partitioning theory and methodology
RSC Advances, (6): 47771-47801. 2016. 10.1039/c6ra04656h
- Manzetti, S.; Patek, M.
The accurate wavefunction of the active space of the rhenium dimer resolved using the ab initio Brueckner coupled-cluster method
Structural Chemistry, (27): 1071-1080. 2016. 10.1007/s11224-015-0726-1
- Manzoni, V.; Coutinho, K.; Canuto, S.
An insightful approach for understanding solvatochromic reversal
Chemical Physics Letters, (655): 30-34. 2016. 10.1016/j.cplett.2016.05.028
- Mao, Y. Z.; Horn, P. R.; Mardirossian, N.; Head-Gordon, T.; Skylaris, C. K.; Head-Gordon, M.
Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation
Journal of Chemical Physics, (145) 2016. 10.1063/1.4959125
- Marin-Luna, M.; Alkorta, I.; Elguero, J.
A computational study on (PH₂X)(2) (center dot+) homodimers involving intermolecular two-center three-electron bonds
Structural Chemistry, (27): 753-762. 2016. 10.1007/s11224-015-0617-5
- Marin-Luna, M.; Alkorta, I.; Elguero, J.
Cooperativity in Tetrel Bonds
Journal of Physical Chemistry A, (120): 648-656. 2016. 10.1021/acs.jpca.5b11876
- Marin-Luna, M.; Alkorta, I.; Elguero, J.
Interaction of beryllium derivatives with N-methylated DNA bases: 9-methylguanine and 1-methylcytosine
Tetrahedron, (72): 1978-1983. 2016. 10.1016/j.tet.2016.02.062
- Marino, T.; Russo, N.
Structure and properties of a copper-mediated nucleobase pair from density functional theory investigation
Inorganica Chimica Acta, (452): 194-198. 2016. 10.1016/j.ica.2016.03.047

- Markovic, Z.; Dorovic, J.; Dimitric Markovic, J. M.; Biocanin, R.; Amic, D.
Comparative density functional study of antioxidant activity of the hydroxybenzoic acids and their anions
Turkish Journal of Chemistry, (40): 499-509. 2016. 10.3906/kim-1503-89
- Markovic, Z.; Jeremic, S.; Markovic, J. D.; Pirkovic, M. S.; Amic, D.
Influence of structural characteristics of substituents on the antioxidant activity of some anthraquinone derivatives
Computational and Theoretical Chemistry, (1077): 25-31. 2016. 10.1016/j.comptc.2015.10.004
- Marshall, B. D.; Chapman, W. G.
THERMODYNAMIC PERTURBATION THEORY FOR ASSOCIATING MOLECULES
Advances in Chemical Physics, Vol 160, (160): 1-47. 2016.
- Marsusi, F.; Qasemnazhand, M.
Sila-fullerenes: promising chemically active fullerene analogs
Nanotechnology, (27) 2016. 10.1088/0957-4484/27/27/275704
- Martin, B.; Autschbach, J.
Kohn-Sham calculations of NMR shifts for paramagnetic 3d metal complexes: protocols, delocalization error, and the curious amide proton shifts of a high-spin iron(II) macrocycle complex
Physical Chemistry Chemical Physics, (18): 21051-21068. 2016. 10.1039/c5cp07667f
- Martinez, Y. B.; Pirani, L. S. R.; Erben, M. F.; Boese, R.; Reuter, C. G.; Vishnevskiy, Y. V.; Mitzel, N. W.; Della Vedova, C. O.
Structures of Trichloromethyl Thiocyanate, CCl_3SCN , in Gaseous and Crystalline State
Chemphyschem, (17): 1463-1467. 2016. 10.1002/cphc.201600063
- Martinez, Y. B.; Reuter, C. G.; Vishnevskiy, Y. V.; Bava, Y. B.; Picone, A. L.; Romano, R. M.; Stammler, H. G.; Neumann, B.; Mitzel, N. W.; Della Vedova, C. O.
Structural Analysis of Perfluoropropanoyl Fluoride in the Gas, Liquid, and Solid Phases
Journal of Physical Chemistry A, (120): 2420-2430. 2016. 10.1021/acs.jpca.6b00424
- Mart'yanov, T. P.; Klimenko, L. S.; Ushakov, E. N.
Oligoether Derivatives of 1-Phenoxyanthraquinone: Synthesis, Photochromism, and Complex Formation with Metal Cations
Russian Journal of Organic Chemistry, (52): 1126-1136. 2016. 10.1134/s1070428016080066
- Marvi, M.; Raissi, H.; Ghiassi, H.
Effects of the HCN adsorption on the structural and electronic parameters of the beryllium oxide nanotube
Structural Chemistry, (27): 557-571. 2016. 10.1007/s11224-015-0585-9
- Masoodi, H. R.; Bagheri, S.; Abareghi, M.
The effects of tautomerization and protonation on the adenine-cytosine mismatches: a density functional theory study
Journal of Biomolecular Structure & Dynamics, (34): 1143-1155. 2016. 10.1080/07391102.2015.1072734
- Masoodi, H. R.; Bagheri, S.; Ranjbar, M.
Theoretical study of cooperativity between hydrogen bond-hydrogen bond, halogen bond-halogen bond and hydrogen bond-halogen bond in ternary FX center dot center dot center diazine center dot center dot center XF (X = H and Cl) complexes
Molecular Physics, (114): 3464-3474. 2016. 10.1080/00268976.2016.1236992
- Masoodi, H. R.; Bagheri, S.; Saeednia, S.; Mohammadi, M.; Raeisipoor, A. R.
The influence of substituents on cooperativity between CH center dot center dot center pi and N center dot center dot center H hydrogen bonds in a T-shaped configuration: X-benzeneaSyen(FH center dot center dot center pyrazine center dot center dot center HF) complexes as a working model
Structural Chemistry, (27): 1521-1530. 2016. 10.1007/s11224-016-0777-y
- Matczak, P.

Intramolecular C-H center dot center dot center dot H-C Contacts in Diheteroaryl Ketones and Thioketones: A Theoretical Analysis
Bulletin of the Chemical Society of Japan, (89): 92-102. 2016. 10.1246/bcsj.20150229

Matczak, P.; Domagala, M.; Domagala, S.
Conformers of diheteroaryl ketones and thioketones: a quantum chemical study of their properties and fundamental intramolecular energetic effects
Structural Chemistry, (27): 855-869. 2016. 10.1007/s11224-015-0643-3

Mathammal, R.; Sangeetha, K.; Sangeetha, M.; Mekala, R.; Gadheeja, S.
Molecular structure, vibrational, UV, NMR, HOMO-LUMO, MEP, NLO, NBO analysis of 3,5 di tert butyl 4 hydroxy benzoic acid
Journal of Molecular Structure, (1120): 1-14. 2016. 10.1016/j.molstruc.2016.05.008

Matsubara, T.; Ito, T.
Quantum Mechanical and Molecular Dynamics Studies of the Reaction Mechanism of the Nucleophilic Substitution at the Si Atom
Journal of Physical Chemistry A, (120): 2636-2646. 2016. 10.1021/acs.jpca.6b02308

Matsuki, N.; Inoue, Y.; Mori, T.
Orbital Control of Photochemical Rearrangement of 4-Aryl-1,1-dicyano-1-butenes through the Hyperconjugative Substitution on the Linker Chain
Journal of Physical Chemistry Letters, (7): 4957-4961. 2016. 10.1021/acs.jpclett.6b02632

Matsumiya, M.; Yamada, T.; Murakami, S.; Kohno, Y.; Tsunashima, K.
Evaluation of the Extraction Properties and Stability of Extracted Rare Earth Complexes in Ionic Liquid Extraction System Using beta-Diketone
Solvent Extraction and Ion Exchange, (34): 454-468. 2016. 10.1080/07366299.2016.1207393

Matta, C. F.; Sadjadi, S.; Braden, D. A.; Frenking, G.
The Barrier to the Methyl Rotation in Cis-2-Butene and its Isomerization Energy to Trans-2-Butene, Revisited
Journal of Computational Chemistry, (37): 143-154. 2016. 10.1002/jcc.24223

Maturana, R. G.; Munoz-Castro, A.
Insights into metal-ligand and metal-metal interaction in coinage metal triangles. Insights of d(10)-d(10), d(10)-d(8) and d(8)-d(8) contacts from Au3In(CH3N=COCH3)(3) (n=2, 4, 6) via relativistic DFT calculations
Chemical Physics Letters, (651): 34-38. 2016. 10.1016/j.cplett.2016.03.013

Matxain, J. M.; Asua, J. M.; Ruiperez, F.
Design of new disulfide-based organic compounds for the improvement of self-healing materials
Physical Chemistry Chemical Physics, (18): 1758-1770. 2016. 10.1039/c5cp06660c

Maxwell, P.; Pendas, A. M.; Popelier, P. L. A.
Extension of the interacting quantum atoms (IQA) approach to B3LYP level density functional theory (DFT)
Physical Chemistry Chemical Physics, (18): 20986-21000. 2016. 10.1039/c5cp07021j

Mazurek, A.
ELECTRON DONOR ACCEPTOR DESCRIPTORS OF THE SINGLE AND DOUBLE BONDED SUBSTITUENT AND HETEROATOM INCORPORATION EFFECTS. A REVIEW
Acta Poloniae Pharmaceutica, (73): 269-283. 2016.

Mbarki, M.; Oettinghaus, M.; Raabe, G.
Quantum-chemical Ab Initio Calculations on the Donor Acceptor Complex Pyridine Borabenzene (C5H5N BC5H5) (vol 69, pg 583, 2016)
Australian Journal of Chemistry, (69): 583-+. 2016. 10.1071/ch13407_co

McDowell, S. A. C.

A computational study of simultaneous cation/anion interactions in model clusters containing all-cis 1,2,3-trifluorocyclopropane (F3C3H3) and all-cis 1,2,3,4-tetrafluorobutane (F4C4H4)
Chemical Physics Letters, (665): 105-110. 2016. 10.1016/j.cplett.2016.10.055

McDowell, S. A. C.
Cooperativity and bond breakage in model X-center dot center dot center dot H3P center dot center dot center dot YZ (X = F, Cl, YZ = HF, ClF, LiF, BeH2) complexes
Chemical Physics Letters, (658): 12-19. 2016. 10.1016/j.cplett.2016.06.007

McDowell, S. A. C.; Fiedler, C. S.
A computational study of beryllium-bonded H2Be center dot center dot center dot FNgH/FKrCl (Ng = Ar, Kr) dyads and their intermolecular interactions with the model nucleophiles F-, NH3 and NCH
Computational and Theoretical Chemistry, (1084): 150-156. 2016. 10.1016/j.comptc.2016.03.028

McDowell, S. A. C.; Maynard, S. J.
A computational study of model hydrogen-, halogen-, beryllium- and magnesium-bonded complexes of aziridine derivatives
Molecular Physics, (114): 1609-1618. 2016. 10.1080/00268976.2016.1142128

McKee, M. L.
A New Nitrogenase Mechanism Using a CFe8S9 Model: Does H-2 Elimination Activate the Complex to N-2 Addition to the Central Carbon Atom?
Journal of Physical Chemistry A, (120): 754-764. 2016. 10.1021/acs.jpca.5b10384

Megala, M.; Rajkumar, B. J. M.
Theoretical study of anthoxanthin dyes for dye sensitized solar cells (DSSCs)
Journal of Computational Electronics, (15): 557-568. 2016. 10.1007/s10825-016-0791-8

Mehio, N.; Ivanov, A. S.; Ladshaw, A. P.; Dai, S.; Bryantsev, V. S.
Theoretical Study of Oxovanadium(IV) Complexation with Formamidoximate: Implications for the Design of Uranyl-Selective Adsorbents
Industrial & Engineering Chemistry Research, (55): 4231-4240. 2016. 10.1021/acs.iecr.5b03398

Mehio, N.; Ivanov, A. S.; Williams, N. J.; Mayes, R. T.; Bryantsev, V. S.; Hancock, R. D.; Dai, S.
Quantifying the binding strength of salicyaldoxime-uranyl complexes relative to competing salicyaldoxime-transition metal ion complexes in aqueous solution: a combined experimental and computational study
Dalton Transactions, (45): 9051-9064. 2016. 10.1039/c6dt00116e

Mehmood, A.; Janesko, B. G.
The electron delocalization range in stretched bonds
International Journal of Quantum Chemistry, (116): 1783-1795. 2016. 10.1002/qua.25225

Mei, L.; Wu, Q. Y.; Yuan, L. Y.; Wang, L.; An, S. W.; Xie, Z. N.; Hu, K. Q.; Chai, Z. F.; Burns, P. C.; Shi, W. Q.
An Unprecedented Two-Fold Nested Super-Polyrotaxane: SulfateDirected Hierarchical Polythreading Assembly of Uranyl Polyrotaxane Moieties
Chemistry-a European Journal, (22): 11329-11338. 2016. 10.1002/chem.201601506

Melekhova, A. A.; Novikov, A. S.; Bokach, N. A.; Avdonceva, M. S.; Kukushkin, V. Y.
Characterization of Cu-ligand bonds in tris-pyrazolylmethane isocyanide copper(I) complexes based upon combined X-ray diffraction and theoretical study
Inorganica Chimica Acta, (450): 140-145. 2016. 10.1016/j.ica.2016.05.031

Melo, T.; Domingues, P.; Ferreira, R.; Milic, I.; Fedorova, M.; Santos, S. M.; Segundo, M. A.; Domingues, M. R. M.
Recent Advances on Mass Spectrometry Analysis of Nitrated Phospholipids
Analytical Chemistry, (88): 2622-2629. 2016. 10.1021/acs.analchem.5b03407

Memarian, H. R.; Ebrahimi, S.; Rudbari, H. A.; Sabzyan, H.; Nardo, V. M.

Inter- and intramolecular interactions in 2,3-dihydroquinazolin-4(1H)-ones: molecular structure and conformational analysis
Journal of the Iranian Chemical Society, (13): 1395-1404. 2016. 10.1007/s13738-016-0854-6

Memarian, H. R.; Sabzyan, H.; Sanchooli, E.
DFT study of the molecular structure of 4,6-diary1-2-oxo-1,2,3,4-tetrahydropyrimidines
Computational and Theoretical Chemistry, (1093): 9-19. 2016. 10.1016/j.comptc.2016.07.019

Mendoza, F.; Gomez, H.; Lluch, J. M.; Masgrau, L.
alpha 1,4-N-Acetylhexosaminyltransferase EXTL2: The Missing Link for Understanding Glycosidic Bond Biosynthesis with Retention of Configuration
ACS Catalysis, (6): 2577-2589. 2016. 10.1021/acscatal.5b02945

Meng, Q. X.; Su, P. Y.; Wang, F.; Zhu, S. H.
Substituent effect and ligand exchange control the reactivity in ruthenium(II)-catalyzed hydroacylation of isoprenes and aldehydes: A DFT study
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s021963361650019x

Meng, Q. X.; Wang, F.
Mechanisms and reactivity differences for the cobalt-catalyzed enantioselective intramolecular hydroacylation of ketones and alkenes: insights from density functional calculations
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2930-3

Menges, F. S.; Craig, S. M.; Totsch, N.; Bloomfield, A.; Ghosh, S.; Kruger, H. J.; Johnson, M. A.
Capture of CO₂ by a Cationic Nickel(I) Complex in the Gas Phase and Characterization of the Bound, Activated CO₂ Molecule by Cryogenic Ion Vibrational Predissociation Spectroscopy
Angewandte Chemie-International Edition, (55): 1282-1285. 2016. 10.1002/anie.201507965

Menkir, M. G.; Lee, S. L.
Intramolecular hydroarylation of aryl propargyl ethers catalyzed by indium: the mechanism of the reaction and identifying the catalytic species
Organic & Biomolecular Chemistry, (14): 6508-6516. 2016. 10.1039/c6ob00877a

Menkir, M. G.; Srinivasadesikan, V.; Lee, S. L.
The role of cesium fluoride in aryl propargyl ether Claisen rearrangement and its mechanistic elucidation: a theoretical study
Structural Chemistry, (27): 1383-1393. 2016. 10.1007/s11224-016-0758-1

Mercy, M.; de Leeuw, N. H.; Bell, R. G.
Mechanisms of CO₂ capture in ionic liquids: a computational perspective
Faraday Discussions, (192): 479-492. 2016. 10.1039/c6fd00081a

Mert, B. D.; Mert, M. E.; Kardas, G.; Yazici, B.
The experimental and quantum chemical investigation for two isomeric compounds as aminopyrazine and 2-amino-pyrimidine against mild steel corrosion
Anti-Corrosion Methods and Materials, (63): 369-376. 2016. 10.1108/acmm-12-2014-1480

Metsala, A.; Zari, S.; Kanger, T.
Aza-Michael Reactions of Isatin Imines: Deeper Insight and Origin of the Stereoselectivity
Chemcatchem, (8): 2961-2967. 2016. 10.1002/cctc.201600584

Metz, A.; Plothe, R.; Glowacki, B.; Koszalkowski, A.; Schechenbach, M.; Beringer, A.; Rosener, T.; de Vasconcellos, J. M.; Haase, R.; Florke, U.; Hoffmann, A.; Herres-Pawlis, S.
Zinc Chloride Complexes with Aliphatic and Aromatic Guanidine Hybrid Ligands and Their Activity in the Ring-Opening Polymerisation of D,L-Lactide
European Journal of Inorganic Chemistry: 4974-4987. 2016. 10.1002/ejic.201600870

Mewes, S. A.; Mewes, J. M.; Dreuw, A.; Plasser, F.

Excitons in poly(para phenylene vinylene): a quantum-chemical perspective based on high-level ab initio calculations
Physical Chemistry Chemical Physics, (18): 2548-2563. 2016. 10.1039/c5cp07077e

Miao, C. Q.; Yu, D. H.; Huang, L. N.; Zhang, S. M.; Yu, L. G.; Zhang, P. Y.
Synthesis of 1,3,5-Tris(phenylamino) Benzene Derivatives and Experimental and Theoretical Investigations of Their Antioxidation Mechanism
Industrial & Engineering Chemistry Research, (55): 1819-1826. 2016. 10.1021/acs.iecr.5b04295

Michalski, J.; Kucharska, E.; Sasiadek, W.; Lorenc, J.; Hanuza, J.
Excited states of selected hydrazo-compounds on the example of 5-nitro-2-(2-phenylhydrazinyl)pyridine and its 3-, 4-or 6-methyl isomers
Journal of Molecular Structure, (1123): 80-91. 2016. 10.1016/j.molstruc.2016.06.019

Mielcarek, A.; Dolega, A.
Weak hydrogen bonding interaction S-H center dot center dot center dot O=C studied by FT-IR spectroscopy and DFT calculations
Journal of Molecular Structure, (1103): 217-223. 2016. 10.1016/j.molstruc.2015.09.032

Mikhaylov, V. N.; Sorokoumov, V. N.; Korvinson, K. A.; Novikov, A. S.; Balova, I. A.
Synthesis and Simple Immobilization of Palladium(II) Acyclic Diaminocarbene Complexes on Polystyrene Support as Efficient Catalysts for Sonogashira and Suzuki-Miyaura Cross-Coupling
Organometallics, (35): 1684-1697. 2016. 10.1021/acs.organomet.6b00144

Mikherdov, A. S.; Kinzhakov, M. A.; Novikov, A. S.; Boyarskiy, V. P.; Boyarskaya, I. A.; Dar'in, D. V.; Starova, G. L.; Kukushkin, V. Y.
Difference in Energy between Two Distinct Types of Chalcogen Bonds Drives Regioisomerization of Binuclear (Diaminocarbene)Pd-II Complexes
Journal of the American Chemical Society, (138): 14129-14137. 2016. 10.1021/jacs.6b09133

Mikulas, T. C.; Chen, M. Y.; Fang, Z. T.; Peterson, K. A.; Andrews, L.; Dixon, D. A.
Structures and Properties of the Products of the Reaction of Lanthanide Atoms with H₂O: Dominance of the plus II Oxidation State
Journal of Physical Chemistry A, (120): 793-804. 2016. 10.1021/acs.jpca.5b11215

Mingos, D. M. P.
The Chemical Bond: Lewis and Kossel's Landmark Contribution
Chemical Bond I: 100 Years Old and Getting Stronger, (169): 1-56. 2016. 10.1007/430_2015_203

Miradji, F.; Virot, F.; Souvi, S.; Cantrel, L.; Louis, F.; Vallet, V.
Thermochemistry of Ruthenium Oxyhydroxide Species and Their Impact on Volatile Speciations in Severe Nuclear Accident Conditions
Journal of Physical Chemistry A, (120): 606-614. 2016. 10.1021/acs.jpca.5b11142

Miranda-Rojas, S.; Salazar-Molina, R.; Kastner, J.; Arratia-Perez, R.; Mendizabal, F.
Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials
RSC Advances, (6): 4458-4468. 2016. 10.1039/c5ra21964g

Mirats, A.; Ali-Torres, J.; Rodriguez-Santiago, L.; Sodupe, M.
Stability of transient Cu(+)_n beta (1-16) species and influence of coordination and peptide configuration on superoxide formation
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1836-6

Mirtamizdoust, B.; Bienko, D. C.; Hanifehpour, Y.; Tiekkink, E. R. T.; Yilmaz, V. T.; Talemi, P.; Joo, S. W.
Preparation of a Novel Nano-scale Lead (II) Zig-Zag Metal-Organic Coordination Polymer with Ultrasonic Assistance: Synthesis, Crystal Structure, Thermal Properties, and NBO Analysis of Pb(mu-2-pinh)N-3 H₂O (n)
Journal of Inorganic and Organometallic Polymers and Materials, (26): 819-828. 2016. 10.1007/s10904-016-0385-8

Mirzaeva, I. V.; Mainichev, D. A.; Kozlova, S. G.

A Localized Molecular Orbital Study of the Halogen Substitution Effect on Rh-103 NMR Shielding in Cp^{}RhX₂ (2), Where X = Cl, Br, or I*
Journal of Physical Chemistry A, (120): 1944-1949. 2016. 10.1021/acs.jpca.6b00882

Mishra, P.; Verma, K.; Bawari, D.; Viswanathan, K. S.
Does borazine-water behave like benzene-water? A matrix isolation infrared and ab initio study
Journal of Chemical Physics, (144) 2016. 10.1063/1.4953793

Mitin, A. V.
ATOMIC STRUCTURE OF THE HIGHEST MOLECULAR ORBITALS OF SMALL TETRA-HEME CYTOCHROME C 1M1P
Journal of Structural Chemistry, (57): 637-641. 2016. 10.1134/s0022476616040016

Mitra, I.; Mukherjee, S.; Reddy, B. V. P.; Dasgupta, S.; Bose, K. J. C.; Mukherjee, S.; Linert, W.; Moi, S. C.
Benzimidazole based Pt(II) complexes with better normal cell viability than cisplatin: synthesis, substitution behavior, cytotoxicity, DNA binding and DFT study
RSC Advances, (6) 2016. 10.1039/c6ra17788c

Miura, Y.; Hoshino, Y.; Seto, H.
Glycopolymers Nanobiotechnology
Chemical Reviews, (116): 1673-1692. 2016. 10.1021/acs.chemrev.5b00247

Miura-Akagi, P. M.; Nakashige, M. L.; Maile, C. K.; Oshiro, S. M.; Gurr, J. R.; Yoshida, W. Y.; Royappa, A. T.; Krause, C. E.; Rheingold, A. L.; Hughes, R. P.; Cain, M. F.
Synthesis of a Tris(phospholealkene)phosphine Ligand and Fundamental Organometallic Reactions on Its Sterically Shielded Metal Complexes
Organometallics, (35): 2224-2231. 2016. 10.1021/acs.organomet.6b00250

Moc, J.
Adsorption, Dissociation, and Dehydrogenation of Water Monomer and Water Dimer on the Smallest 3D Aluminum Particle. The O-H Dissociation Barrier Disappears for the Dimer
Journal of Physical Chemistry A, (120): 8725-8737. 2016. 10.1021/acs.jpca.6b08278

Mohajeri, A.; Haghshenas, F.
Global reactivity and site selectivity of (TiO₂)_n nanoclusters (n=5-10) toward hydrogen peroxide
Materials Chemistry and Physics, (183): 326-333. 2016. 10.1016/j.matchemphys.2016.08.035

Mohamdi, M.; Bensouilah, N.; Abdaoui, M.
Investigation of charge transfer complexes formed between (S,S)-bis- N,N-sulfonyl bis-L-phenylalanine dimethylester donor with tetracyanoethylene and chloranil as pi-acceptors: Experimental and DFT studies
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500097

Mohammadpour, M.; Zborowski, K. K.; Heidarpoor, S.; Zuchowski, G.; Proniewicz, L. M.
Modeling of stability and properties of anionic and cationic tautomers of the 3-hydroxypyridin-4-one system
Computational and Theoretical Chemistry, (1078): 96-103. 2016. 10.1016/j.comptc.2015.12.023

Mohapatra, C.; Kundu, S.; Paesch, A. N.; Herbst-Irmer, R.; Stalke, D.; Andrade, D. M.; Frenking, G.; Roesky, H. W.
The Structure of the Carbene Stabilized Si₂H₂ May Be Equally Well Described with Coordinate Bonds as with Classical Double Bonds
Journal of the American Chemical Society, (138): 10429-10432. 2016. 10.1021/jacs.6b07361

Mollenhauer, D.; Gaston, N.
Phosphine passivated gold clusters: how charge transfer affects electronic structure and stability
Physical Chemistry Chemical Physics, (18): 29686-29697. 2016. 10.1039/c6cp04562f

Momeni, S.; Farrokhnia, M.; Karimi, S.; Nabipour, I.
Copper hydroxide nanostructure-modified carbon ionic liquid electrode as an efficient voltammetric sensor for detection of metformin: a theoretical and experimental study
Journal of the Iranian Chemical Society, (13): 1027-1035. 2016. 10.1007/s13738-016-0816-z

- Momeni, Z.; Ebrahimi, A.
The influence of CH ... broken vertical bar pi interaction on hydrogen bonding ability of -CONH₂ functional group of benzamide
Structural Chemistry, (27): 1199-1209. 2016. 10.1007/s11224-016-0745-6
- Momin, M. I. K.; Koobanally, N. A.; Honarpourvar, B.
Imidazole-based Derivatives as Potential Anti-platelet Inhibitors: DFT and Molecular Docking Study
Letters in Drug Design & Discovery, (13): 888-896. 2016. 10.2174/1570180813666160517162937
- Mompean, M.; Nogales, A.; Ezquerro, T. A.; Laurents, D. V.
Complex System Assembly Underlies a Two-Tiered Model of Highly Delocalized Electrons
Journal of Physical Chemistry Letters, (7): 1859-1864. 2016. 10.1021/acs.jpclett.6b00699
- Mondal, B.; Bhattacharya, S.; Ghosh, S.
Heterometallic boride clusters of group 6 and 9 transition metals
Journal of Organometallic Chemistry, (819): 147-154. 2016. 10.1016/j.jorgchem.2016.06.027
- Mondal, B.; Bhattacharyya, M.; Varghese, B.; Ghosh, S.
Hypo-electronic triple-decker sandwich complexes: synthesis and structural characterization of ((CpMo)-Mo-star)(2){mu-eta(6):eta(6)-B4H4E-Ru(CO)(3)} (E = S, Se, Te or Ru(CO)(3) and Cp-star = eta(5)-C5Me5)
Dalton Transactions, (45): 10999-11007. 2016. 10.1039/c6dt01214k
- Mondal, K. C.; Roy, S.; Dittrich, B.; Andrada, D. M.; Frenking, G.; Roesky, H. W.
A Triatomic Silicon(0) Cluster Stabilized by a Cyclic Alkyl(amino) Carbene
Angewandte Chemie-International Edition, (55): 3158-3161. 2016. 10.1002/anie.201511019
- Mondal, S.; Cabellos, J. L.; Pan, S.; Osorio, E.; Torres-Vega, J. J.; Tiznado, W.; Restrepo, A.; Merino, G.
10-pi-Electron arenes a la carte: structure and bonding of the E-(C_nH_n)-E (n=6) (E = Ca, Sr, Ba; n=6-8) complexes
Physical Chemistry Chemical Physics, (18): 11909-11918. 2016. 10.1039/c6cp00671j
- Mondal, S.; Mugesh, G.
Biomimetic deiodination of thyroid hormones and iodothyronamines - a structure-activity relationship study
Organic & Biomolecular Chemistry, (14): 9490-9500. 2016. 10.1039/c6ob01375a
- Mondal, S.; Mugesh, G.
Conformational Flexibility and Halogen Bonding in Thyroid Hormones and Their Metabolites
Crystal Growth & Design, (16): 5896-5906. 2016. 10.1021/acs.cgd.6b00945
- Mondal, S.; Osorio, E.; Pan, S.; Cabellos, J. L.; Martinez, S.; Florez, E.; Merino, G.
Why CpAl-Cr(CO)(5) is linear while CpIn-Cr(CO)(5) is not? Understanding the structure and bonding of the CpE-Cr(CO)(5) (E = Group 13 element) complexes
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1993-7
- Mondal, T.; De, S.; Maity, B.; Koley, D.
Exploring the Oxidative-Addition Pathways of Phenyl Chloride in the Presence of Pd-II Abnormal N-Heterocyclic Carbene Complexes: A DFT Study
Chemistry-a European Journal, (22): 15778-15790. 2016. 10.1002/chem.201602735
- Mondragon-Solorzano, G.; Sierra-Alvarez, R.; Lopez-Honorato, E.; Barroso-Flores, J.
In silico design of calixarene-based arsenic acid removal agents
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (85): 169-174. 2016. 10.1007/s10847-016-0617-0
- Montagna, M.; Jeanvoine, Y.; Spezia, R.; Bodo, E.
Structure, Stability, and Electronic Properties of Dimethyl Sulfoxide and Dimethyl Formamide Clusters Containing Th⁴⁺
Journal of Physical Chemistry A, (120): 4778-4788. 2016. 10.1021/acs.jpca.5b12007

- Montazerozohori, M.; Masoudiasl, A.; Doert, T.; Seykens, H.
Structural and computational study of some new nano-structured Hg(II) compounds: a combined X-ray, Hirshfeld surface and NBO analyses
RSC Advances, (6): 21396-21412. 2016. 10.1039/c5ra22899a
- Montejo-Valencia, B. D.; Salcedo-Perez, J. L.; Curet-Arana, M. C.
DFT Study of Closed and Open Sites of BEA, FAU, MFI, and BEC Zeolites Substituted with Tin and Titanium
Journal of Physical Chemistry C, (120): 2176-2186. 2016. 10.1021/acs.jpcc.5b09815
- Montero-Campillo, M. M.; Lamsabhi, A.; Mo, O.; Yanez, M.
Photochemical Behavior of Beryllium Complexes with Subporphyrazines and Subphthalocyanines
Journal of Physical Chemistry A, (120): 4845-4852. 2016. 10.1021/acs.jpca.5b12374
- Moosavi-Tekyeh, Z.; Taherian, F.; Tayyari, S. F.
Intramolecular hydrogen bonding in 5-nitrosalicylaldehyde: IR spectrum and quantum chemical calculations
Journal of Molecular Structure, (1111): 185-192. 2016. 10.1016/j.molstruc.2016.01.084
- Morales-Meza, S.; Perez-Peralta, N.; Sanchez-Castro, M. E.; Sanchez, M.
Theoretical study of penta- and heteropentadienyl beryllium complexes coordinated to hydrogen molecules
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3110-1
- Moreira, A. A. G.; De Lima-Neto, P.; Caetano, E. W. S.; Barroso-Neto, I. L.; Freire, V. N.
Computational electronic structure of the bee killer insecticide imidacloprid
New Journal of Chemistry, (40): 10353-10362. 2016. 10.1039/c6nj02743a
- Moreira, L.; Calbo, J.; Arago, J.; Illescas, B. M.; Nierengarten, I.; Delavaux-Nicot, B.; Orti, E.; Martin, N.; Nierengarten, J. F.
Conjugated Porphyrin Dimers: Cooperative Effects and Electronic Communication in Supramolecular Ensembles with C-60
Journal of the American Chemical Society, (138): 15359-15367. 2016. 10.1021/jacs.6b07250
- Morera-Boado, C.; Gonzalez, M. M.; Miranda-Quintana, R. A.; Suarez, M.; Martinez-Alvarez, R.; Martin, N.; de la Vega, J. M. G.
Theoretical Study on the Mechanism of the Thermal Retro-Cycloaddition of Isoxazolinofullerenes
Journal of Physical Chemistry A, (120): 8830-8842. 2016. 10.1021/acs.jpca.6b07297
- Morera-Boado, C.; Reyes-Retana, J. A.; Avila, M.; Mikosch, H.
First principle calculations of the adsorption of molecular H-2 in Cu Fe(CN)(5)NO metal nitroprussides. An insight into H-2-host interactions
Computational Materials Science, (117): 54-64. 2016. 10.1016/j.commatsci.2016.01.026
- Morera-Boado, C.; Reyes-Retana, J. A.; Avila, M.; Zumeta, I.; Mikosch, H.; Rodriguez, C.
First principle calculations on the adsorption of molecular H-2 in the largest pore of Co Fe(CN)(5)NO and Ni Fe(CN)(5)NO metal nitroprussides. Effect of the charged cavities on the adsorption and H-2-host interactions
Computational Materials Science, (114): 102-111. 2016. 10.1016/j.commatsci.2015.12.019
- Morgenstern, A.; Eberhart, M.
Bond dissociation energies from the topology of the charge density using gradient bundle analysis
Physica Scripta, (91) 2016. 10.1088/0031-8949/91/2/023012
- Moridi, M.; Shekarsaraei, S.; Hadipour, N. L.
DFT Studies of NH-Cl Hydrogen Bond of Amino Acid Hydrochloride Salts in Ion Channels
Acta Chimica Slovenica, (63): 241-250. 2016. 10.17344/acs.2015.1927
- Morita, H.; Van Beylen, M.
New Vistas on the Anionic Polymerization of Styrene in Non-Polar Solvents by Means of Density Functional Theory
Polymers, (8) 2016. 10.3390/polym8100371
- Morosaki, T.; Fujii, T.
Synthesis of phosphorus- and sulfur-stabilized carbone (Me) Ph2P -> C <- SP2 (= NMe)

Phosphorus Sulfur and Silicon and the Related Elements, (191): 159-162. 2016. 10.1080/10426507.2015.1114488

Morozov, A. N.; Chatfield, D. C.

How the Proximal Pocket May Influence the Enantiospecificities of Chloroperoxidase-Catalyzed Epoxidations of Olefins
International Journal of Molecular Sciences, (17) 2016. 10.3390/ijms17081297

Morzyk-Ociepa, B.; Dysz, K.; Turowska-Tyrk, I.; Michalska, D.

New trans-dichloropalladium(II) complexes of 7-azaindole: Crystal and molecular structures, FT-IR, FT-Raman and DFT studies

Journal of Molecular Structure, (1103): 202-211. 2016. 10.1016/j.molstruc.2015.09.019

Mousavi, M.; Pahlavan, F.; Oldham, D.; Abdollahi, T.; Fini, E. H.

Alteration of intermolecular interactions between units of asphaltene dimers exposed to an amide-enriched modifier
RSC Advances, (6): 53477-53492. 2016. 10.1039/c6ra07506a

Moussa, J.; Chamoreau, L. M.; Gullo, M. P.; Degli Esposti, A.; Barbieri, A.; Amouri, H.

Induced phosphorescence from Pt → Ag and Ag(I)center dot center dot center dot Ag(I) metallophilic interactions in benzenedithiolatodiimine-Pt-2/Ag-2 clusters: a combined experimental and theoretical investigation
Dalton Transactions, (45): 2906-2913. 2016. 10.1039/c5dt03702f

Mu, W. H.; Fang, D. C.; Xia, S. Y.; Cheng, R. J.; Chass, G. A.

Multi-Pathway Consequent Chemoselectivities of CpRuCl(PPh₃)(2)/MeI-Catalysed Norbornadiene Alkyne Cycloadditions
Chemistry-a European Journal, (22): 15396-15403. 2016. 10.1002/chem.201603173

Mu, X. L.; Yang, X. D.; Zhang, D. J.; Liu, C. B.

Theoretical study of the reaction of chitosan monomer with 2,3-epoxypropyl-trimethyl quaternary ammonium chloride catalyzed by an imidazolium-based ionic liquid
Carbohydrate Polymers, (146): 46-51. 2016. 10.1016/j.carbpol.2016.03.032

Mudliar, N. H.; Sadhu, B.; Pettiwala, A. M.; Singh, P. K.

Evaluation of an Ultrafast Molecular Rotor, Auramine O, as a Fluorescent Amyloid Marker
Journal of Physical Chemistry B, (120): 10496-10507. 2016. 10.1021/acs.jpcb.6b07807

Mukaiyama, T.; Uchimaru, T.; Hayashi, Y.

The DFT Calculation with NBO Analysis of E/Z Enamines Derived from alpha-Alkoxyaldehyde with Pyrrolidine
Bulletin of the Chemical Society of Japan, (89): 455-459. 2016. 10.1246/bcsj.20150382

Mukherjee, S.; Mitra, I.; Reddy, B. V. P.; Mahata, S.; Bose, K. J. C.; Dasgupta, S.; Linert, W.; Moi, S. C.

Cytotoxic, DNA binding and drug reservoir property of Pt(II)-sulfur complexes: In-vitro kinetics, mechanism with bio-relevant molecules in aqueous medium and a theoretical approach
Polyhedron, (119): 84-97. 2016. 10.1016/j.poly.2016.08.024

Mukherjee, V.; Yadav, T.

Conformational study of neutral histamine monomer and their vibrational spectra
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (165): 167-175. 2016.
10.1016/j.saa.2016.04.041

Mukhopadhyay, A.

Interplay between C-H center dot center dot center dot O, O-H center dot center dot center dot X (X = C, F, Cl) and H-O center dot center dot center dot Y (C, Cl, F) interactions in methane-water and halogen substituted methane-water complexes: Theoretical investigations of structure and energy
Computational and Theoretical Chemistry, (1083): 19-30. 2016. 10.1016/j.comptc.2016.03.004

Muller, G.; Voronova, K.; Sztaray, B.; Meioni, G.

Rotamers and Migration: Investigating the Dissociative Photoionization of Ethylenediamine
Journal of Physical Chemistry A, (120): 3906-3916. 2016. 10.1021/acs.jpca.6b03516

- Muniz, J.; Castillo, R.; Robles, J. B.; Sansores, E.
Density Functional Theory Study of the Reactivity and Electronic Structure of the Transesterification of Triacetin in Biodiesel Production via a Sulfated Zirconia Heterogeneous Catalysis
International Journal of Quantum Chemistry, (116): 988-999. 2016. 10.1002/qua.25116
- Munro, A. M.; Chandler, C.; Garling, M.; Chai, D.; Popovich, V.; Lystrom, L.; Kilina, S.
Phenyldithiocarbamate Ligands Decompose During Nanocrystal Ligand Exchange
Journal of Physical Chemistry C, (120): 29455-29462. 2016. 10.1021/acs.jpcc.6b08247
- Munzer, J. E.; Ona-Burgos, P.; Arrabal-Campos, F. M.; Neumuller, B.; Tonner, R.; Fernandez, I.; Kuzu, I.
Difluoroboreonium Cation Stabilized by Hexaphenyl-Carbodiphosphorane: A Concise Study on the Molecular and Electronic Structure of (Ph₃P)(2)C(sic)BF₂ BF₄
European Journal of Inorganic Chemistry: 3852-3858. 2016. 10.1002/ejic.201600519
- Murugavel, S.; Stephen, C.; Subashini, R.; Reddy, H. R.; AnanthaKrishnan, D.
Synthesis, crystal structure investigation, spectroscopic characterizations and DFT computations on a novel 1-(2-chloro-4-phenylquinolin-3-yl)ethanone
Journal of Molecular Structure, (1122): 134-145. 2016. 10.1016/j.molstruc.2016.05.095
- Murugavel, S.; Velan, V. V.; Kannan, D.; Bakthadoss, M.
Experimental and computational approaches of a novel methyl (2E)-2-{ N-(2-formylphenyl)(4-methylbenzene)sulfonamido methyl}-3-(4-chlorophenyl)prop-2-enoate: A potential antimicrobial agent and an inhibition of penicillin-binding protein
Journal of Molecular Structure, (1115): 33-54. 2016. 10.1016/j.molstruc.2016.02.084
- Murugavel, S.; Velan, V. V.; Kannan, D.; Bakthadoss, M.
Synthesis, crystal structure analysis, spectral investigations, DFT computations, Biological activities and molecular docking of methyl(2E)-2-{ N-(2-formylphenyl)(4-methylbenzene)sulfonamido methyl}-3-(4-fluorophenyl)prop-2-enoate, a potential bioactive agent
Journal of Molecular Structure, (1108): 150-167. 2016. 10.1016/j.molstruc.2015.11.047
- Mushtaque, M.; Jahan, M.; Ali, M.; Khan, M. S.; Khan, M. S.; Sahay, P.; Kesarwani, A.
Synthesis, characterization, molecular docking, DNA binding, cytotoxicity and DFT studies of 1-(4-methoxyphenyl)-3-(pyridine-3-ylmethyl)thiourea
Journal of Molecular Structure, (1122): 164-174. 2016. 10.1016/j.molstruc.2016.05.087
- Nabavizadeh, S. M.; Sepehrpour, H.; Jamshidi, M.; Hosseini, F. N.; Owczarzak, A. M.; Kubicki, M.
Binuclear organoplatinum(II) complexes with double bis(diphenylphosphino) acetylene bridges: Synthesis, X-ray structure determination, electronic structures and DFT calculations
Journal of Organometallic Chemistry, (808): 34-41. 2016. 10.1016/j.jorganchem.2016.02.012
- Naderi, F.
Structures and electronic properties of C₁₂Si₈X₈ (X = H, F, and Cl)
Russian Journal of Physical Chemistry A, (90): 1385-1390. 2016. 10.1134/s0036024416070220
- Nagata, T.; Miyajima, K.; Mafune, F.
Gold Atoms Supported on Gas-Phase Cerium Oxide Cluster Ions: Stable Stoichiometry and Reactivity with CO
Journal of Physical Chemistry A, (120): 7624-7633. 2016. 10.1021/acs.jpca.6b08257
- Nair, S. S.; Prakash, S.; Vignesh, D.; Suvitha, A.; Venkataramanan, N. S.
Structure, stability and reactivity of neutral and charged monomeric chromium oxide clusters
Computational and Theoretical Chemistry, (1082): 58-66. 2016. 10.1016/j.comptc.2016.02.018
- Nakajima, T.; Noda, S.; Sakamoto, M.; Matsui, A.; Nakamae, K.; Kure, B.; Ura, Y.; Tanase, T.
Oxidative addition of an aromatic ortho C-H bond of tetraphosphine to asymmetric diiridium(I) centres
Dalton Transactions, (45): 4747-4761. 2016. 10.1039/c5dt04725k
- Nakanishi, W.; Tsubomoto, Y.; Hayashi, S.

Nature of S₂Se₂ sigma(4c-6e) at naphthalene 1,8-positions and models, elucidated by QTAIM dual functional analysis
RSC Advances, (6): 93195-93204. 2016. 10.1039/c6ra17767k

Nakata, K.; Siehl, H. U.; Maas, G.; Fujio, M.

Computational study of substituent effects on the gas-phase stabilities of N-phenylguanidinium ions
Journal of Physical Organic Chemistry, (29): 741-749. 2016. 10.1002/poc.3569

Nakayama, T.; Uno, B.

Concerted two-proton-coupled electron transfer from catechols to superoxide via hydrogen bonds
Electrochimica Acta, (208): 304-309. 2016. 10.1016/j.electacta.2016.05.034

Nakazawa, T.; Kaji, Y.

A density functional theory investigation of the reactions of Fe and FeO₂ with O₂
Computational Materials Science, (117): 455-467. 2016. 10.1016/j.commatsci.2016.01.023

Nakhaei, E.; Nowroozi, A.

On the performance of resonance assisted hydrogen bond theory in malonaldehyde derivatives
Computational and Theoretical Chemistry, (1096): 27-32. 2016. 10.1016/j.comptc.2016.09.029

Nandi, G.; Chilukuri, B.; Hipps, K. W.; Mazur, U.

Surface directed reversible imidazole ligation to nickel(II) octaethylporphyrin at the solution/solid interface: a single molecule level study
Physical Chemistry Chemical Physics, (18): 20819-20829. 2016. 10.1039/c6cp04454a

Narayanan, R.; Velloth, A.; Kurahashi, T.; Fujii, H.; Hada, M.

The Origin of Relative Stability of Di-mu-oxo M-M Chiral Salen Complexes M-M = Ti(TV)-Ti(IV), V(IV)-V(IV), Cr(IV)-Cr(IV), and Mn(IV) Mn(IV) : A Quantum-Chemical Analysis
Bulletin of the Chemical Society of Japan, (89): 447-454. 2016. 10.1246/bcsj.20150393

Naseri, M.; Fotouhi, L.; Ehsani, A.; Babaei, F.

Physicoelectrochemical properties of facilely electrosynthesized reduced graphene oxide/p-type conductive polymer nanocomposite film
New Journal of Chemistry, (40): 2565-2573. 2016. 10.1039/c5nj02969d

Nasr, A.; Winkler, A.; Tamm, M.

Anionic N-heterocyclic carbenes: Synthesis, coordination chemistry and applications in homogeneous catalysis
Coordination Chemistry Reviews, (316): 68-124. 2016. 10.1016/j.ccr.2016.02.011

Naumkin, F. Y.; Wales, D. J.

Trapping of hydrogen atoms inside small beryllium clusters and their ions
Chemical Physics Letters, (659): 282-288. 2016. 10.1016/j.cplett.2016.07.054

Nauroozi, D.; Orthaber, A.

The Heavier Analogues of Alkenes: A Theoretical Comparison of Unsaturated Group 15/14 Systems
European Journal of Inorganic Chemistry: 709-717. 2016. 10.1002/ejic.201500848

Neil, F.; Chelsea, M.; D'Acchioli, J.; Webster, A.

Oxidation states naturally: A natural bond orbital study
Abstracts of Papers of the American Chemical Society, (251) 2016.

Nepal, B.; Scheiner, S.

Building a Better Halide Receptor: Optimum Choice of Spacer, Binding Unit, and Halosubstitution
Chemphyschem, (17): 836-844. 2016. 10.1002/cphc.201501149

Nepal, B.; Scheiner, S.

Enhancing the Reduction Potential of Quinones via Complex Formation
Journal of Organic Chemistry, (81): 4316-4324. 2016. 10.1021/acs.joc.6b00755

- Nepal, B.; Scheiner, S.
NX center dot center dot center dot Y halogen bonds. Comparison with NH center dot center dot center dot Y H-bonds and CX center dot center dot center dot Y halogen bonds
Physical Chemistry Chemical Physics, (18): 18015-18023. 2016. 10.1039/c6cp03771b
- Neto, I.; Andrade, J.; Fernandes, A. S.; Reis, C. P.; Salunke, J. K.; Priimagi, A.; Candeias, N. R.; Rijo, P.
Multicomponent Petasis-borono Mannich Preparation of Alkylaminophenols and Antimicrobial Activity Studies
Chemmedchem, (11): 2015-2023. 2016. 10.1002/cmdc.201600244
- Newberry, R. W.; Orke, S. J.; Raines, R. T.
n ->pi Interactions Are Competitive with Hydrogen Bonds*
Organic Letters, (18): 3614-3617. 2016. 10.1021/acs.orglett.6b01655
- Newberry, R. W.; Raines, R. T.
A prevalent intraresidue hydrogen bond stabilizes proteins
Nature Chemical Biology, (12): 1084-+. 2016. 10.1038/nchembio.2206
- Ngo, P. D.; Mansoorabadi, S. O.; Frey, P. A.
Serine Protease Catalysis: A Computational Study of Tetrahedral Intermediates and Inhibitory Adducts
Journal of Physical Chemistry B, (120): 7353-7359. 2016. 10.1021/acs.jpcb.6b04089
- Nguyen, A. L.; Wang, M. D.; Bobadova-Parvanova, P.; Do, Q.; Zhou, Z. H.; Fronczek, F. R.; Smith, K. M.; Vicente, M. G. H.
Synthesis and properties of B-cyano-BODIPYs
Journal of Porphyrins and Phthalocyanines, (20): 1409-1419. 2016. 10.1142/s108842461650125x
- Nguyen, T. A. N.; Huynh, T. P. L.; Tran, T. H.; Pham, V. T.; Duong, T. Q.; Dang, T. H.
Structures and Bonding Situation of Iron Complexes of Group-13 Half-Sandwich ECp (E = B to TI) Based on DFT Calculations*
Zeitschrift fur Anorganische und Allgemeine Chemie, (642): 609-617. 2016. 10.1002/zaac.201600104
- Nhu, Q.; Nguyen, N.; Tantillo, D. J.
When To Let Go-Diradical Intermediates from Zwitterionic Transition State Structures?
Journal of Organic Chemistry, (81): 5295-5302. 2016. 10.1021/acs.joc.6b00533
- Nhung, N. T. A.; Loan, H. T. P.; Quang, D. T.; Sy, T. D.; Hiep, D. T.
Structural variations and chemical bonding in platinum complexes of Group 14 heavier tetrelene homologues (germylene to plumbylene)
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (55): 269-276. 2016.
- Nie, H. C.; Su, Y. C.; Zhang, M. T.; Song, Y.; Leone, A.; Taylor, L. S.; Marsac, P. J.; Li, T. L.; Byrn, S. R.
Solid-State Spectroscopic Investigation of Molecular Interactions between Clofazimine and Hypromellose Phthalate in Amorphous Solid Dispersions
Molecular Pharmaceutics, (13): 3964-3975. 2016. 10.1021/acs.molpharmaceut.6b00740
- Nieto, P.; Gunther, A.; Berden, G.; Oomens, J.; Dopfer, O.
IRMPD Spectroscopy of Metalated Flavins: Structure and Bonding of Lumiflavin Complexes with Alkali and Coinage Metal Ions
Journal of Physical Chemistry A, (120): 8297-8308. 2016. 10.1021/acs.jpca.6b08281
- Nijesh, K.; De, S.; Parameswaran, P.
Homopolar dihydrogen bonding in ligand stabilized diberyllium hydride complexes, Be-2(CH₃)(2)H₂L₂ (L = H-, CO, N-heterocyclic carbene and CN-)
Dalton Transactions, (45): 7836-7846. 2016. 10.1039/c5dt04293c
- Nikolaienko, T. Y.; Bulavin, L. A.; Hovorun, D. M.
Can we treat ab initio atomic charges and bond orders as conformation-independent electronic structure descriptors?
RSC Advances, (6): 74785-74796. 2016. 10.1039/c6ra17055b

- Nikoofard, H.; Sargolzaei, M.; Kia, B.; Amin, A. H.
DFT study of conjugational electronic structures of aminoalkyl end-capped oligothiophenes up to octamers
Comptes Rendus Chimie, (19): 646-653. 2016. 10.1016/j.crci.2016.01.004
- Nizovtsev, A. S.
Search for aromatic anions in the P2E3- ($E = N, P, As, Sb, Bi$) series
Physical Chemistry Chemical Physics, (18): 16084-16087. 2016. 10.1039/c6cp02241c
- Noei, M.; Salari, A. A.; Baei, M. T.; Hajizadeh, F.; Asl, J. K.; Taghartapeh, M. R.
Theoretical study of fMet-tRNA and fAla-tRNA structures by using quantum calculation
Arabian Journal of Chemistry, (9): S1019-S1028. 2016. 10.1016/j.arabjc.2011.11.010
- Nonnenmacher, M.; Buck, D. M.; Kunz, D.
Experimental and theoretical investigations on the high-electron donor character of pyrido-annelated N-heterocyclic carbenes
Beilstein Journal of Organic Chemistry, (12): 1884-1896. 2016. 10.3762/bjoc.12.178
- Nori-Shargh, D.; Mousavi, S. N.; Tale, R.; Yahyaei, H.
Hyperconjugative interactions are the main responsible for the anomeric effect: a direct relationship between the hyperconjugative anomeric effect, global hardness and zero-point energy
Structural Chemistry, (27): 1753-1768. 2016. 10.1007/s11224-016-0791-0
- Novak, M.; Dostal, L.; Turek, J.; Alonso, M.; De Proft, F.; Ruzicka, A.; Jambor, R.
Spontaneous Double Hydrometallation Induced by NM Coordination in Organometallic Hydrides of Group 14 Elements
Chemistry-a European Journal, (22): 5620-5628. 2016. 10.1002/chem.201504947
- Novikov, A. S.; Kuznetsov, M. L.; Rocha, B. G. M.; Pombeiro, A. J. L.; Shul'pin, G. B.
Oxidation of olefins with H₂O₂ catalysed by salts of group III metals (Ga, In, Sc, Y and La): epoxidation versus hydroperoxidation
Catalysis Science & Technology, (6): 1343-1356. 2016. 10.1039/c5cy01367d
- Novotny, J.; Bazzi, S.; Marek, R.; Kozelka, J.
Lone-pair-pi interactions: analysis of the physical origin and biological implications
Physical Chemistry Chemical Physics, (18): 19472-19481. 2016. 10.1039/c6cp01524g
- Nowroozi, A.; Rahmani, S.; Eshraghi, A.; Shayan, K.
A comparative study of two-ring resonance-assisted hydrogen bond systems
Structural Chemistry, (27): 829-838. 2016. 10.1007/s11224-015-0637-1
- Nozawa, R.; Tanaka, H.; Cha, W. Y.; Hong, Y.; Hisaki, I.; Shimizu, S.; Shin, J. Y.; Kowalczyk, T.; Irle, S.; Kim, D.; Shinokubo, H.
Stacked antiaromatic porphyrins
Nature Communications, (7) 2016. 10.1038/ncomms13620
- Nunes, C. M.; Pinto, S. M. V.; Reva, I.; Fausto, R.
On the Photochemistry of 1,2-Benzisoxazole: Capture of Elusive Spiro-2H-azirine and Ketenimine Intermediates
European Journal of Organic Chemistry: 4152-4158. 2016. 10.1002/ejoc.201600668
- Nwankwo, H. U.; Ateba, C. N.; Olasunkanmi, L. O.; Adekunle, A. S.; Isabirye, D. A.; Onwudiwe, D. C.; Ebenso, E. E.
Synthesis, Characterization, Antimicrobial Studies and Corrosion Inhibition Potential of 1,8-dimethyl-1,3,6,8,10,13-hexaaazacyclotetradecane: Experimental and Quantum Chemical Studies
Materials, (9) 2016. 10.3390/ma9020107
- Nzikou, V. D. N.; Scheiner, S.
Catalysis of the Aza-Diels-Alder Reaction by Hydrogen and Halogen Bonds
Journal of Organic Chemistry, (81): 2589-2597. 2016. 10.1021/acs.joc.6b00344
- Nzikou, V. D. N.; Scheiner, S.

Comparison of pi-hole tetrel bonding with sigma-hole halogen bonds in complexes of XCN (X = F, Cl, Br, I) and NH3
Physical Chemistry Chemical Physics, (18): 3581-3590. 2016. 10.1039/c5cp07545a

Ochoa-Resendiz, D.; Batista-Romero, F. A.; Hernandez-Lamoneda, R.
Communication: Evidence of halogen bonds in clathrate cages
Journal of Chemical Physics, (145) 2016. 10.1063/1.4966644

Ocola, E. J.; Laane, J.
Spectroscopic and Theoretical Study of the Intramolecular i pi-Type Hydrogen Bonding and Conformations of 2-Cyclohexen-1-ol
Journal of Physical Chemistry A, (120): 74-80. 2016. 10.1021/acs.jpca.5b11114

Ohkawa, T.; Kuramoto, K.
Theoretical study of CO and O₂ adsorption and CO oxidation on linear-shape gold molecules (LGM(n)) (n=2, 4, 8, 16, and 24)
AIP Advances, (6) 2016. 10.1063/1.4962824

Ohsato, T.; Okuno, Y.; Ishida, S.; Iwamoto, T.; Lee, K. H.; Lin, Z. Y.; Yamashita, M.; Nozaki, K.
A Potassium Diboryllithate: Synthesis, Bonding Properties, and the Deprotonation of Benzene
Angewandte Chemie-International Edition, (55): 11426-11430. 2016. 10.1002/anie.201605005

Oliveira, B. G.
THE FORMATION OF THE pi center dot center dot center dot center dot H, F center dot center dot center dot center dot H AND C center dot center dot center dot center dot H HYDROGEN BONDS ON THE C₂H₂ center dot center dot center dot center dot HF, C₂H₂ center dot center dot center dot center dot 2(HF) AND C₂H₂ center dot center dot center dot center dot 3(HF) COMPLEXES
Quimica Nova, (39): 320-327. 2016. 10.5935/0100-4042.20160021

Oliveira, B. G.
The interaction strength of intermolecular systems formed by NaH center dot center dot center dot 2(HF) and NaH center dot center dot center dot center dot 4(HF): Hydrogen bonds, dihydrogen bonds and halogen-hydride bonds
Comptes Rendus Chimie, (19): 995-1002. 2016. 10.1016/j.crci.2016.03.015

Oliveira, T. S. M.; Freitas, V. L. S.; da Silva, M.
Energetic insights on two dye key molecules: N-methylphenotheniazine and N-methylphenoxyazine
Journal of Chemical Thermodynamics, (94): 7-15. 2016. 10.1016/j.jct.2015.10.013

Omelchenko, I. V.; Shishkin, O. V.; Gorb, L.; Leszczynski, J.
Aromaticity and conformational flexibility of five-membered monoheterocycles: pyrrole-like and thiophene-like structures
Structural Chemistry, (27): 101-109. 2016. 10.1007/s11224-015-0707-4

Omidyan, R.; Iravani, M.
Excited-state intramolecular proton transfer and photoswitching in hydroxyphenyl-imidazopyridine derivatives: A theoretical study
Journal of Chemical Physics, (145) 2016. 10.1063/1.4967199

Oppermann, A.; Dick, R.; Wehrhahn, C.; Florke, U.; Herres-Pawlis, S.; Henkel, G.
Copper(I) Thiolate Heteroadamantane Cage Structures with Relevance to Metalloproteins
European Journal of Inorganic Chemistry: 3744-3755. 2016. 10.1002/ejic.201600247

O'Reilly, R. J.; Karton, A.
A Dataset of Highly Accurate Homolytic N-Br Bond Dissociation Energies Obtained by Means of W2 Theory
International Journal of Quantum Chemistry, (116): 52-60. 2016. 10.1002/qua.25024

Orenha, R. P.; Gregorio, L. R. S.; Galembek, S. E.
Computational study of the interaction between NO, NO+, and NO- with H₂O
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3148-0

- Orr, V. L.; Esselman, B. J.; Dorman, P. M.; Amberger, B. K.; Guzei, I. A.; Woods, R. C.; McMahon, R. J.
Millimeter-Wave Spectroscopy, X-ray Crystal Structure, and Quantum Chemical Studies of Diketene: Resolving Ambiguities Concerning the Structure of the Ketene Dimer
Journal of Physical Chemistry A, (120): 7753-7763. 2016. 10.1021/acs.jpca.6b07610
- Ortega, D. E.; Nguyen, Q. N. N.; Tantillo, D. J.; Toro-Labbe, A.
The catalytic effect of the NH₃ base on the chemical events in the caryolene-forming carbocation cascade
Journal of Computational Chemistry, (37): 1068-1081. 2016. 10.1002/jcc.24294
- Ortega, P. G. R.; Montejo, M.; Gonzalez, J. J. L.
Hyperconjugative and Electrostatic Interactions as Anomeric Triggers in Archetypical 1,4-Dioxane Derivatives
Chemphyschem, (17): 530-540. 2016. 10.1002/cphc.201500989
- Osipova, E. S.; Belkova, N. V.; Epstein, L. M.; Filippov, O. A.; Kirkina, V. A.; Titova, E. M.; Rossin, A.; Peruzzini, M.; Shubina, E. S.
Dihydrogen Bonding and Proton Transfer from MH and OH Acids to Group 10 Metal Hydrides ((PCP)-P-tBu)MH (PCP)-P-tBu = kappa(3)-2,6-(tBu(2)PCH(2))(2)C₆H₃; M = Ni, Pd
European Journal of Inorganic Chemistry: 1415-1424. 2016. 10.1002/ejic.201600034
- Osorio, E.; Ferraro, F.; Hadad, C. Z.; Rabanal-Leon, W. A.; Tiznado, W.
Insights on the structural and electronic properties of ScC_n⁺, YC_n⁺, LaC_n⁺ (n=3-6) systems
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1976-8
- Padhye, R.; Aquino, A. J. A.; Tunega, D.; Pantoya, M. L.
Effect of Polar Environments on the Aluminum Oxide Shell Surrounding Aluminum Particles: Simulations of Surface Hydroxyl Bonding and Charge
ACS Applied Materials & Interfaces, (8): 13926-13933. 2016. 10.1021/acsami.6b02665
- Padilla-Campos, L.; Zarate, R. A.
ELECTRONIC AND STRUCTURAL PROPERTIES OF 5-HYDROXY-7-METOXYFLAVANONE: A THEORETICAL APPROACH
Journal of the Chilean Chemical Society, (61): 3267-3272. 2016. 10.4067/s0717-97072016000400023
- Padole, M. C.; Deshpande, P. A.
Tailoring Surface Adsorption and Reactivity of Fullerene-Based Compounds: A Theoretical Probe into C-2-Gas-Fullerene Surface Interactions
Journal of Physical Chemistry C, (120): 12654-12665. 2016. 10.1021/acs.jpcc.6b03747
- Pagacz-Kostrzewska, M.; Saldyka, M.; Wierzejewska, M.; Khomenko, D. M.; Doroschuk, R. O.
Theoretical DFT and matrix isolation FTIR studies of 2-(1,2,4-triazolyl) phenol isomers
Chemical Physics Letters, (657): 156-161. 2016. 10.1016/j.cplett.2016.06.005
- Pahlavan, F.; Pakiari, A. H.
DFT study of the chlorine promotion effect on the ethylene adsorption over iron clusters
Journal of Molecular Graphics & Modelling, (66): 58-66. 2016. 10.1016/j.jmgm.2016.03.009
- Pairas, G. N.; Tsoungas, P. G.
H-Bond: The Chemistry-Biology H-Bridge
Chemistryselect, (1): 4520-4532. 2016. 10.1002/slct.201600770
- Pakiari, A. H.; Dehghanpisheh, E.
The electronic structure of nanoparticle: theoretical study of small Cobalt clusters (Co (n), n=2-5) (part A)
Structural Chemistry, (27): 583-593. 2016. 10.1007/s11224-015-0588-6
- Pakiari, A. H.; Shariati, S.
Geometry and electronic structure of ultrafine/nanoparticle chromium clusters (Cr-n, n=2-5) and their interaction with oxygen (triplet) and ethylene molecules: A DFT-NBO study
Computational and Theoretical Chemistry, (1084): 169-178. 2016. 10.1016/j.comptc.2016.03.032
- Pal, A.; Vanka, K.

Small Molecule Activation by Constrained Phosphorus Compounds: Insights from Theory
Inorganic Chemistry, (55): 558-565. 2016. 10.1021/acs.inorgchem.5b01074

Pal, P.; Konar, S.; Lama, P.; Das, K.; Bauza, A.; Frontera, A.; Mukhopadhyay, S.
On the Importance of Noncovalent Carbon-Bonding Interactions in the Stabilization of a 1D Co(II) Polymeric Chain as a Precursor of a Novel 2D Coordination Polymer
Journal of Physical Chemistry B, (120): 6803-6811. 2016. 10.1021/acs.jpcb.6b04046

Pal, S.; Drover, M. W.; Patrick, B. O.; Love, J. A.
Enhancing Reactivity of Directly iObservable B-H-Pt Interactions through Conformational Rigidity
European Journal of Inorganic Chemistry: 2403-2408. 2016. 10.1002/ejic.201501305

Palafox, M. A.; Rastogi, V. K.
6-Aminouracil: Geometries and spectra in the isolated state and in the solid state simulation. A comparison with 5-aminouracil
Journal of Molecular Structure, (1108): 482-495. 2016. 10.1016/j.molstruc.2015.12.004

Palafox, M. A.; Rastogi, V. K.
Density Functional Computations on 6-Aminouracil: Effect of Amino Group in the 6th Position on the Watson-Crick Base Pair Uridine-Adenosine
Australian Journal of Chemistry, (69): 881-889. 2016. 10.1071/ch15793

Palanivel, U.; Lakshmi pathi, S.
Hydrogen bonds in Zif268 proteins - a theoretical perspective
Journal of Biomolecular Structure & Dynamics, (34): 1607-1624. 2016. 10.1080/07391102.2015.1085903

Pan, S.; Ghara, M.; Ghosh, S.; Chattaraj, P. K.
Noble gas bound beryllium chromate and beryllium hydrogen phosphate: a comparison with noble gas bound beryllium oxide
RSC Advances, (6): 92786-92794. 2016. 10.1039/c6ra20232b

Pan, Y. R.; Li, X. M.; Ji, J. Y.; Wang, Q. W.
Synthesis, Crystal Structure, and Theoretical Calculations of Two Cobalt, Nickel Coordination Polymers with 5-Nitroisophthalic Acid and Bis(imidazol) Ligands
Australian Journal of Chemistry, (69): 1296-1304. 2016. 10.1071/ch16110

Pandey, J.; Prajapati, P.; Shimpi, M. R.; Tandon, P.; Velaga, S. P.; Srivastava, A.; Sinha, K.
Studies of molecular structure, hydrogen bonding and chemical activity of a nitrofurantoin-L-proline cocrystal: a combined spectroscopic and quantum chemical approach
RSC Advances, (6): 74135-74154. 2016. 10.1039/c6ra13035f

Pandey, K. K.
Relativistic DFT calculations of structure and Sn-119 NMR chemical shifts for bent M-Sn-C bonding in Power's metalostannyles of chromium, molybdenum, tungsten and iron and diaryl stannyles
Journal of Organometallic Chemistry, (815-816): 23-34. 2016. 10.1016/j.jorgchem.2016.05.006

Pandey, K. K.
Theoretical insights into the relative bonding of normal and abnormal N-heterocyclic carbenes in PdCl₂(NHCR)(2) and PdCl₂(NHCR)(aNHC(R)) (R=H, Ph, Mes)
International Journal of Quantum Chemistry, (116): 537-546. 2016. 10.1002/qua.25077

Pandey, K. K.; Vishwakarma, R.; Patidar, S. K.
Theoretical insights into the nature of bonding in group 13-group 15 compounds RE=E' R (E = B-Tl; E' = N-Bi; R = Me, Ph, Ar): Bonding energy analysis
Computational and Theoretical Chemistry, (1076): 23-31. 2016. 10.1016/j.comptc.2015.11.019

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

Does the occurrence of resonance (by the delocalization of radical/cationic/anionic charges) induce the existence of intramolecular halogen-halogen contacts?
RSC Advances, (6): 66870-66878. 2016. 10.1039/c6ra14270b

Panek, J. J.; Blaziak, K.; Jeziorska, A.
Hydrogen bonds in quinoline N-oxide derivatives: first-principle molecular dynamics and metadynamics ground state study
Structural Chemistry, (27): 65-75. 2016. 10.1007/s11224-015-0720-7

Pang, R.; Yu, L. J.; Zhang, M.; Tian, Z. Q.; Wu, D. Y.
DFT Study of Hydrogen-Bonding Interaction, Solvation Effect, and Electric-Field Effect on Raman Spectra of Hydrated Proton
Journal of Physical Chemistry A, (120): 8273-8284. 2016. 10.1021/acs.jpca.6b07064

Pankratov, A. N.; Fedotova, O. V.; Ozerova, A. G.; Mazhukina, O. A.; Strashilina, I. V.
Structure and stabilization factors of the 2-aminobenzimidazolium-3,3'-(phenylmethylene)- bis(4-hydroxy-2H-chromen-2-one) anion associate in the system 4-hydroxy-2H-chromen-2-one-benzimidazol-2-amine-benzaldehyde
Russian Journal of Organic Chemistry, (52): 1326-1334. 2016. 10.1134/s107042801609013x

Papayannis, D. K.; Papavasileiou, K. D.; Melissas, V. S.
Investigation of bromine atom transfer mechanism from an alkyl bromide molecule to an O-bonded alkyl group in a FAU zeolite by the ONIOM method
Microporous and Mesoporous Materials, (226): 1-9. 2016. 10.1016/j.micromeso.2015.12.034

Paranthaman, S.; Moon, J.; Hong, K.; Kim, J.; Kim, D. E.; Kim, J.; Kim, T. K.
Reactivity of molecular oxygen with aluminum clusters: Density functional and Ab Initio molecular dynamics simulation study
International Journal of Quantum Chemistry, (116): 547-554. 2016. 10.1002/qua.25080

Park, J. W.; Rhee, Y. M.
Electric Field Keeps Chromophore Planar and Produces High Yield Fluorescence in Green Fluorescent Protein
Journal of the American Chemical Society, (138): 13619-13629. 2016. 10.1021/jacs.6b06833

Park, J. W.; Rhee, Y. M.
Emission shaping in fluorescent proteins: role of electrostatics and pi-stacking
Physical Chemistry Chemical Physics, (18): 3944-3955. 2016. 10.1039/c5cp07535a

Parveen, S.; Al-Alshaikh, M. A.; Panicker, C. Y.; El-Emam, A. A.; Salian, V. V.; Narayana, B.; Sarojini, B. K.; van Alsenoy, C.
Spectroscopic investigations and molecular docking study of (2E)-1-(4-Chlorophenyl)-3- 4-(propan-2-yl)phenyl prop-2-en-1-one using quantum chemical calculations
Journal of Molecular Structure, (1120): 317-326. 2016. 10.1016/j.molstruc.2016.05.030

Parveen, S. S.; Al-Alshaikh, M. A.; Panicker, C. Y.; El-Emam, A. A.; Arisoy, M.; Temiz-Arpaci, O.; Van Alsenoy, C.
*Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial and antimicrobial studies of 5-ethylsulphonyl-2-(*p*-aminophenyl)benzoxazole*
Journal of Molecular Structure, (1115): 94-104. 2016. 10.1016/j.molstruc.2016.02.057

Parveen, S. S.; Al-Alshaikh, M. A.; Panicker, C. Y.; El-Emam, A. A.; Narayana, B.; Saliyan, V. V.; Sarojini, B. K.; Van Alsenoy, C.
*Vibrational and structural observations and molecular docking study on 1-(3-(4-chlorophenyl)-5- 4-(propan-2-yl)phenyl -4,5-dihydro-1*H*-*p*-pyrazol -1-yl}-ethanone*
Journal of Molecular Structure, (1112): 136-146. 2016. 10.1016/j.molstruc.2016.02.018

Parvin, N.; Pal, S.; Rojisha, V. C.; De, S.; Parameswaran, P.; Khan, S.
Comparing Nucleophilicity of Heavier Heteroleptic Amidinato-Amido Tetrellyenes: An Experimental and Theoretical Study
Chemistryselect, (1): 1991-1995. 2016. 10.1002/slct.201600656

Parvini, E.; Vatanparast, M.; Vessally, E.; Bahadori, A.

Is there theoretical evidence for mutual influence between halogen and pnictogen-hydride bonds? An ab initio study
Journal of Chemical Sciences, (128): 1905-1912. 2016. 10.1007/s12039-016-1196-8

Pasban, S.; Raissi, H.; Mollania, F.

Solvent effects on the structural, electronic properties and intramolecular N-H O hydrogen bond strength of 5-aminomethylene-pyrimidine-2,4,6 trion with DFT calculations
Journal of Molecular Liquids, (215): 77-87. 2016. 10.1016/j.molliq.2015.11.038

Passadis, S. S.; Tsiafoulis, C.; Drouza, C.; Tsimpis, A. C.; Miras, H. N.; Keramidas, A. D.; Kabanos, T. A.

Synthesis, Bonding, and Reactivity of Vanadium(IV) Oxido-Fluorido Compounds with Neutral Chelate Ligands of the General Formula cis- V-IV(=O)(F)(LN-N)(2) (+)
Inorganic Chemistry, (55): 1364-1366. 2016. 10.1021/acs.inorgchem.5b02895

Patel, P. D.; Laird, B. B.; Thompson, W. H.

A density functional theory study of ethylene epoxidation catalyzed by niobium-doped silica
Journal of Molecular Catalysis a-Chemical, (424): 1-7. 2016. 10.1016/j.molcata.2016.07.052

Patel, R. N.; Singh, Y.; Singh, Y. P.; Butcher, R. J.; Kamal, A.; Tripathi, I. P.

Copper(II) and nickel(II) complexes with N'-(Z)-phenyl(pyridin-2-yl)methylidene acetohydrazide: Synthesis, crystal structures, DFT calculations and antioxidant effects
Polyhedron, (117): 20-34. 2016. 10.1016/j.poly.2016.05.036

Patel, R. N.; Singh, Y. P.; Singh, Y.; Butcher, R. J.

Synthesis, crystal structure, DFT calculations and superoxide dismutase activity of copper(II) complex with pyridine-2-carboxylic acid
Journal of the Indian Chemical Society, (93): 469-480. 2016.

Patel, R. N.; Singh, Y. P.; Singh, Y.; Butcher, R. J.

Synthesis, crystal structure, DFT computation and bioactivity measurements of copper(II) polypyridyl complexes
Polyhedron, (104): 116-126. 2016. 10.1016/j.poly.2015.11.042

Pathak, D.; Deuri, S.; Phukan, P.

Theoretical Insights on the Interaction of N -Heterocyclic Carbenes with Tetravalent Silicon Reagents
Journal of Physical Chemistry A, (120): 128-138. 2016. 10.1021/acs.jpca.5b08676

Patil, M.; Thiel, W.

Mechanism of Ylide Transfer to Carbonyl Compounds: Density Functional Calculations
European Journal of Organic Chemistry: 830-839. 2016. 10.1002/ejoc.201501073

Paunescu, I.; Medeleanu, M.; Pop, R. O.; Simon, Z.; Costisor, O.

A DFT STUDY ON 2-(HYDROXY-2-BENZYLIDENE)-CYCLOHEXANONE
Revue Roumaine de Chimie, (61): 711-719. 2016.

Pedrick, E. A.; Hrobarik, P.; Seaman, L. A.; Wu, G.; Hayton, T. W.

Synthesis, structure and bonding of hexaphenyl thorium(IV): observation of a non-octahedral structure
Chemical Communications, (52): 689-692. 2016. 10.1039/c5cc08265j

Pejlovas, A. M.; Daly, A. M.; Ashe, A. J.; Kukolich, S. G.

Microwave spectra, molecular structure, and aromatic character of 4a,8a-azaboranaphthalene
Journal of Chemical Physics, (144) 2016. 10.1063/1.4943882

Pell, T. P.; Wilson, D. J. D.; Skelton, B. W.; Dutton, J. L.; Barnard, P. J.

Heterobinietallic N-Heterocyclic Carbene Complexes: A Synthetic, Spectroscopic, and Theoretical Study
Inorganic Chemistry, (55): 6882-6891. 2016. 10.1021/acs.inorgchem.6b00222

Pelzer, S.; Neumann, B.; Stammier, H. G.; Ignat'ev, N.; Hoge, B.

The Bis(pentafluoroethyl)germylene Trimethylphosphane Adduct (C₂F₅)₂GePMe₃: Characterization, Ligand Properties, and Reactivity

Angewandte Chemie-International Edition, (55): 6088-6092. 2016. 10.1002/anie.201601468

Pepin, R.; Laszlo, K. J.; Marek, A.; Peng, B.; Bush, M. F.; Lavanant, H.; Afonso, C.; Turecek, F.
Toward a Rational Design of Highly Folded Peptide Cation Conformations. 3D Gas-Phase Ion Structures and Ion Mobility Characterization
Journal of the American Society for Mass Spectrometry, (27): 1647-1660. 2016. 10.1007/s13361-016-1437-6

Perez, C.; Caballero-Mancebo, E.; Lesarri, A.; Cocinero, E. J.; Alkorta, I.; Suenram, R. D.; Grabow, J. U.; Pate, B. H.
The Conformational Map of Volatile Anesthetics: Enflurane Revisited
Chemistry-a European Journal, (22): 9804-9811. 2016. 10.1002/chem.201601201

Petelski, A. N.; Duarte, D. J. R.; Pamies, S. C.; Peruchena, N. M.; Sosa, G. L.
Intermolecular perturbation in the self-assembly of melamine
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-015-1795-3

Peterson, P. W.; Shevchenko, N.; Breiner, B.; Manoharan, M.; Lufti, F.; Delaune, J.; Kingsley, M.; Kovnir, K.; Alabugin, I. V.
Orbital Crossings Activated through Electron Injection: Opening Communication between Orthogonal Orbitals in Anionic C1-C5 Cyclizations of Enediynes
Journal of the American Chemical Society, (138): 15617-15628. 2016. 10.1021/jacs.6b08540

Petz, W.; Kuzu, I.; Frenking, G.; Andrade, D. M.; Neumuller, B.; Fritz, M.; Munzer, J. E.
Proton Affinities of Cationic Carbone Adducts AC(PPh_3)(2) (+) (A = Halogen, Hydrogen, Methyl) and Unusual Electronic Structures of the Cations and Dications AC(H)(PPh_3)(2) (2+)
Chemistry-a European Journal, (22): 8536-8546. 2016. 10.1002/chem.201600525

Pham, H. T.; Cuong, N. T.; Tam, N. M.; Tung, N. T.
A Systematic Investigation on CrCun Clusters with n=9-16: Noble Gas and Tunable Magnetic Property
Journal of Physical Chemistry A, (120): 7335-7343. 2016. 10.1021/acs.jpca.6b04221

Phi, N. D.; Trung, N. T.; Janssens, E.; Ngan, V. T.
Electron counting rules for transition metal-doped Si-12 clusters
Chemical Physics Letters, (643): 103-108. 2016. 10.1016/j.cplett.2015.11.025

Phien, T. D.; Shlykov, S. A.
N-substituted alkyl- and nonalkylpiperidines: Equatorial, axial or intermediate conformations?
Computational and Theoretical Chemistry, (1087): 26-35. 2016. 10.1016/j.comptc.2016.04.025

Phillips, J. A.
Structural and energetic properties of nitrile-BX3 complexes: substituent effects and their impact on condensed-phase sensitivity
Theoretical Chemistry Accounts, (136) 2016. 10.1007/s00214-016-2035-1

Phipps, M. J. S.; Fox, T.; Tautermann, C. S.; Skylaris, C. K.
Energy Decomposition Analysis Based on Absolutely Localized Molecular Orbitals for Large-Scale Density Functional Theory Calculations in Drug Design
Journal of Chemical Theory and Computation, (12): 3135-3148. 2016. 10.1021/acs.jctc.6b00272

Pick, F. S.; Thompson, J. R.; Savard, D. S.; Leznoff, D. B.; Fryzuk, M. D.
Synthesis of Iron and Cobalt Complexes of a Ferrocene-Linked Diphosphinoamide Ligand and Characterization of a Weak Iron-Cobalt Interaction
Inorganic Chemistry, (55): 4059-4067. 2016. 10.1021/acs.inorgchem.6b00443

Pillegowda, M.; Periyasamy, G.
DFT studies on the influence of ligation on optical and redox properties of bimetallic Au4M2 clusters
RSC Advances, (6): 86051-86060. 2016. 10.1039/c6ra14886g

Pinchuk, D.; Mathew, J.; Kaushansky, A.; Bravo-Zhivotovskii, D.; Apeloig, Y.

Isolation and Characterization, Including by X-ray Crystallography, of Contact and Solvent-Separated Ion Pairs of Silenyl Lithium Species
Angewandte Chemie-International Edition, (55): 10258-10262. 2016. 10.1002/anie.201603640

Pinkas, J.; Cisarova, I.; Gyepes, R.; Kubista, J.; Mach, K.; Horacek, M.
Substituent effects in reduction-induced synthesis of ansa-titanocenes
Transition Metal Chemistry, (41): 143-152. 2016. 10.1007/s11243-015-0006-3

Plaisance, C. P.; Reuter, K.; van Santen, R. A.
Quantum chemistry of the oxygen evolution reaction on cobalt(II,III) oxide - implications for designing the optimal catalyst
Faraday Discussions, (188): 199-226. 2016. 10.1039/c5fd00213c

Plundrich, G. T.; Wadeppohl, H.; Clot, E.; Gade, L. H.
eta(6)-Arene-Zirconium-PNP-Pincer Complexes: Mechanism of Their Hydrogenolytic Formation and Their Reactivity as Zirconium(II) Synthons
Chemistry-a European Journal, (22): 9283-9292. 2016. 10.1002/chem.201601213

Pogany, P.; Kovacs, A.; Visscher, L.; Konings, R. J. M.
Theoretical study of actinide monocarbides (ThC, UC, PuC, and AmC)
Journal of Chemical Physics, (145) 2016. 10.1063/1.4972812

Pokharia, S.; Joshi, R.; Pokharia, M.; Yadav, S. K.; Mishra, H.
A density functional theory insight into the structure and reactivity of diphenyltin(IV) derivative of glycylphenylalanine
Main Group Metal Chemistry, (39): 77-86. 2016. 10.1515/mgmc-2016-0009

Pomogaeva, A. V.; Morokuma, K.; Timoshkin, A. Y.
Trimeric Cluster of Lithium Amidoborane-The Smallest Unit for the Modeling of Hydrogen Release Mechanism
Journal of Computational Chemistry, (37): 1259-1264. 2016. 10.1002/jcc.24316

Pomogaeva, A. V.; Timoshkin, A. Y.
Initial steps for the thermal decomposition of alkaline-earth metal amidoboranes: a cluster approximation
Physical Chemistry Chemical Physics, (18): 31072-31077. 2016. 10.1039/c6cp05835c

Ponce-Vargas, M.; Munoz-Castro, A.
Tiara-like Complexes acting as Iodine Encapsulating Agents: The Role of M center dot center dot center dot center dot I Interactions in M(mu-SCH₂CO₂Me)(2) (8)subset of I-2 (M = Ni, Pd, Pt) Inclusion Compounds
Journal of Physical Chemistry C, (120): 23441-23448. 2016. 10.1021/acs.jpcc.6b08643

Ponec, R.
Modern Theoretical Methods of the Analysis of Molecular Electron Structure
Chemicke Listy, (110): 323-329. 2016.

Popelier, P. L. A.
Quantum Chemical Topology
Chemical Bond II: 100 Years Old and Getting Stronger, (170): 71-117. 2016. 10.1007/430_2015_197

Popoola, S. A.; Al-Saadi, A. A.
Spectroscopic and theoretical evaluation of the metal-olefin interaction in di-mu-chlorobis (1,5-cyclooctadiene) complexes of Ir and Rh
Vibrational Spectroscopy, (86): 109-123. 2016. 10.1016/j.vibspec.2016.06.013

Porto, A. B.; de Oliveira, L. F. C.; Dos Santos, H. F.
Exploring the potential energy surface for reaction of SWCNT with NO₂⁺: A model reaction for oxidation of carbon nanotube in acid solution
Computational and Theoretical Chemistry, (1088): 1-8. 2016. 10.1016/j.comptc.2016.05.002

Posada-Amarillas, A.; Pacheco-Contreras, R.; Morales-Meza, S.; Sanchez, M.; Schon, J. C.

Computational Studies of Stable Hexanuclear Cu_lAg_mAu_n ($l+m+n=6$; $l, m, n > 0$) Clusters
International Journal of Quantum Chemistry, (116): 1006-1015. 2016. 10.1002/qua.25119

Pourmousavi, S. A.; Kanaani, A.; Ghorbani, F.; Damghani, K. K.; Ajloo, D.; Vakili, M.
Synthesis, spectroscopic investigations and computational study of monomeric and dimeric structures of 2-methyl-4-quinolinol
Research on Chemical Intermediates, (42): 1237-1274. 2016. 10.1007/s11164-015-2084-4

Poutas, L. C. D.; Reis, M. C.; Sanz, R.; Lopez, C. S.; Faza, O. N.
A Radical Mechanism for the Vanadium-Catalyzed Deoxydehydration of Glycols
Inorganic Chemistry, (55): 11372-11382. 2016. 10.1021/acs.inorgchem.6b01916

Povolotskii, M. I.; Shablykin, O. V.; Rusanov, E. B.; Rozhenko, A. B.
Molecular and electronic structure of 1,3,2-diazaphosphorinine derivatives
Phosphorus Sulfur and Silicon and the Related Elements, (191): 399-404. 2016. 10.1080/10426507.2015.1091827

Pradeepa, S. J.; Tamilvandan, D.; Boobalan, M. S.; Sundaraganesan, N.
Vibrational and structural observations upon 3-((1H-benzo d imidazol-1-yl)methyl)naphthalen-2-ol from spectral and DFT computing approaches
Journal of Molecular Structure, (1112): 33-44. 2016. 10.1016/j.molstruc.2016.01.026

Prasad, A. A.; Kumar, C. U.; Prakasam, B. A.; Meenakshisundaram, S. P.
Conformational polymorphs of isobutyl-6-amino-5-cyano-2-methyl-4-phenyl-4H-pyran-3-carboxylate: spectroscopic, structural and DFT approach
Acta Crystallographica Section B-Structural Science Crystal Engineering and Materials, (72): 301-309. 2016.
10.1107/s2052520616003310

Prashanth, J.; Reddy, B. V.; Rao, G. R.
Investigation of torsional potentials, molecular structure, vibrational properties, molecular characteristics and NBO analysis of some bipyridines using experimental and theoretical tools
Journal of Molecular Structure, (1117): 79-104. 2016. 10.1016/j.molstruc.2016.03.062

Prathipa, C.; Akilandeswari, L.
Altered torqueselectivity of fluorine in the iron-tricarbonyl-mediated thermal ring opening of 3-fluorocyclobutene: a density-functional exploration
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3125-7

Premkumar, S.; Rekha, T. N.; Asath, R. M.; Jawahar, A.; Mathavan, T.; Benial, A. M. F.
Vibrational spectroscopic, structural and quantum chemical studies on N-phenyl-3-pyridinecarboxamide
Journal of Molecular Structure, (1107): 254-265. 2016. 10.1016/j.molstruc.2015.11.062

Premkumar, S.; Rekha, T. N.; Asath, R. M.; Mathavan, T.; Benial, A. M. F.
Vibrational spectroscopic, molecular docking and density functional theory studies on 2-acetylamo-5-bromo-6-methylpyridine
European Journal of Pharmaceutical Sciences, (82): 115-125. 2016. 10.1016/j.ejps.2015.11.018

Pulido, Y. F.; Suarez, E.; Lopez, R.; Menendez, M. I.
The role of CuCl on the mechanism of dibenzo-p-dioxin formation from poly-chlorophenol precursors: A computational study
Chemosphere, (145): 77-82. 2016. 10.1016/j.chemosphere.2015.11.042

Puskarova, I.; Breza, M.
DFT studies of the effectiveness of p-phenylenediamine antioxidants through their Cu(II) coordination ability
Polymer Degradation and Stability, (128): 15-21. 2016. 10.1016/j.polymdegradstab.2016.02.028

Putau, A.; Brand, H.; Koszinowski, K.
Intermediates Formed in the Reactions of Organocuprates with alpha,beta-Unsaturated Nitriles
Chemistry-a European Journal, (22): 12868-12876. 2016. 10.1002/chem.201602451

- Qi, Q.; Wang, Y. Q.; Dai, Y. Q.; Sun, Y. M.
Spectroscopic properties of carbazolyl and diphenylamino naphthalimide derivatives: the role of solvent and rotational relaxation
Optoelectronics and Advanced Materials-Rapid Communications, (10): 410-416. 2016.
- Qi, Q.; Wang, Y. Q.; Sun, Y. M.
Structural Effect on Absorption and Emission Properties of 1,8-Naphthalimide Derivatives : a DFT Study
Spectroscopy and Spectral Analysis, (36): 3796-3804. 2016. 10.3964/j.issn.1000-0593(2016)11-3796-09
- Qi, T.; Yang, H. Q.; Whitfield, D. M.; Yu, K.; Hu, C. W.
Insights into the Mechanistic Role of Diphenylphosphine Selenide, Diphenylphosphine, and Primary Amines in the Formation of CdSe Monomers
Journal of Physical Chemistry A, (120): 918-931. 2016. 10.1021/acs.jpca.5b10675
- Qi, Y. J.; Zhao, Y. M.; Lu, H. N.; Wang, X. E.; Jin, N. Z.
Exploring molecular flexibility and the interactions of Quercetin derivatives in the active site of alpha-glucosidase using molecular docking and charge density analysis
Computational and Theoretical Chemistry, (1094): 55-68. 2016. 10.1016/j.comptc.2016.09.004
- Qi, Y. J.; Zhao, Y. M.; Wang, X. E.; Lu, H. N.; Jin, N. Z.
Comparative analysis of interactions between the hydroxyridine dicarboxylate derivatives and different proteins by molecular docking and charge density analysis
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500504
- Qin, D. D.; Chen, W.; Tang, X.; Yu, W.; Wu, A. A.; Liao, Y.; Chen, H. B.
Accessing 2-Arylbenzofurans by Cu-2(I)(pip)(2)-Catalyzed Tandem Coupling/Cyclization Reaction: Mechanistic Studies and Application to the Synthesis of Stemofuran A and Moracin M
Asian Journal of Organic Chemistry, (5): 1345-1352. 2016. 10.1002/ajoc.201600321
- Qin, Y. X.; Cui, M. Y.; Ye, Z. H.
Adsorption of ethanol on V2O5 (010) surface for gas-sensing applications: Ab initio investigation
Applied Surface Science, (379): 497-504. 2016. 10.1016/j.apsusc.2016.04.117
- Qiu, S. Y.; Azofra, L. M.; MacFarlane, D. R.; Sun, C. H.
Why is a proton transformed into a hydride by NiFe hydrogenases? An intrinsic reactivity analysis based on conceptual DFT
Physical Chemistry Chemical Physics, (18): 15369-15374. 2016. 10.1039/c6cp00948d
- Qiu, X. J.; Long, J. Y.; Liu, Z. M.; Zhang, B.
Direct imaging of the ultrafast internal conversion in isolated piperidine
Chemical Physics Letters, (645): 133-137. 2016. 10.1016/j.cplett.2015.12.049
- Quinonero, D.; Alkorta, I.; Elguero, J.
Cation-cation and anion-anion complexes stabilized by halogen bonds
Physical Chemistry Chemical Physics, (18): 27939-27950. 2016. 10.1039/c6cp03662g
- Quinonero, D.; Bauza, A.; Sanchez-Sanz, G.; Trujillo, C.; Alkorta, I.; Elguero, J.
Weak interactions within nitryl halide heterodimers
New Journal of Chemistry, (40): 9060-9072. 2016. 10.1039/c6nj01334a
- Rabanal-Leon, W. A.; Murillo-Lopez, J. A.; Arratia-Perez, R.
Insights into bonding interactions and excitation energies of 3d-4f mixed lanthanide transition metal macrocyclic complexes
Physical Chemistry Chemical Physics, (18): 33218-33225. 2016. 10.1039/c6cp07001a
- Racek, T.; Pazurikova, J.; Varekova, R. S.; Geidl, S.; Krenek, A.; Falginella, F. L.; Horsky, V.; Hejret, V.; Koca, J.
NEEMP: software for validation, accurate calculation and fast parameterization of EEM charges

Journal of Cheminformatics, (8) 2016. 10.1186/s13321-016-0171-1

Racine, J.; Hagebaum-Reignier, D.; Carissan, Y.; Humbel, S.

Recasting Wave Functions into Valence Bond Structures: A Simple Projection Method to Describe Excited States
Journal of Computational Chemistry, (37): 771-779. 2016. 10.1002/jcc.24267

Rad, A. S.

Adsorption of mercaptopyridine on the surface of Al- and B-doped graphenes: Theoretical study
Journal of Alloys and Compounds, (682): 345-351. 2016. 10.1016/j.jallcom.2016.05.004

Rad, A. S.

Al-doped graphene as a new nanostructure adsorbent for some halomethane compounds: DFT calculations
Surface Science, (645): 6-12. 2016. 10.1016/j.susc.2015.10.036

Rad, A. S.

Terthiophene as a model sensor for some atmospheric gases: theoretical study
Molecular Physics, (114): 584-591. 2016. 10.1080/00268976.2015.1102348

Rad, A. S.; Ayub, K.

Coordination of nickel atoms with Al₁₂X₁₂ (X = N, P) nanocages enhances H₂ adsorption: A surface study by DFT
Vacuum, (133): 70-80. 2016. 10.1016/j.vacuum.2016.08.017

Rad, A. S.; Ayub, K.

Detailed surface study of adsorbed nickel on Al₁₂N₁₂ nano-cage
Thin Solid Films, (612): 179-185. 2016. 10.1016/j.tsf.2016.05.055

Rad, A. S.; Ayub, K.

Enhancement in hydrogen molecule adsorption on B₁₂N₁₂ nano-cluster by decoration of nickel
International Journal of Hydrogen Energy, (41): 22182-22191. 2016. 10.1016/j.ijhydene.2016.08.158

Rad, A. S.; Ayub, K.

Ni adsorption on Al₁₂P₁₂ nano-cage: A DFT study
Journal of Alloys and Compounds, (678): 317-324. 2016. 10.1016/j.jallcom.2016.03.175

Rad, A. S.; Esfahanian, M.; Ganjian, E.; Tayebi, H. A.

Ab-Initio Study of Physisorption of Hydrogen Cyanide on 2PANI: a Model for Polyaniline Gas Sensor
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics, (230): 1487-1498. 2016. 10.1515/zpch-2015-0645

Rad, A. S.; Zareyee, D.; Foukolaei, V. P.; Moghadas, B. K.; Peyravi, M.

Study on the electronic structure of Al₁₂N₁₂ and Al₁₂P₁₂ fullerene-like nano-clusters upon adsorption of CH₃F and CH₃Cl
Molecular Physics, (114): 3143-3149. 2016. 10.1080/00268976.2016.1220646

Rad, A. S.; Zareyee, D.; Peyravi, M.; Jahanshahi, M.

Surface study of gallium- and aluminum- doped graphenes upon adsorption of cytosine: DFT calculations
Applied Surface Science, (390): 444-451. 2016. 10.1016/j.apsusc.2016.08.065

Radovanovic, L.; Rogan, J.; Poletti, D.; Rodic, M. V.; Begovic, N.

Structural diversity of manganese(II) complexes containing 2,2'-dipyridylamine and benzenedicarboxylates. Conformational analysis of tere-, iso- and phthalate ions: An experimental and quantum chemical approach
Inorganica Chimica Acta, (445): 46-56. 2016. 10.1016/j.ica.2016.02.026

Ragavendran, V.; Muthunatesan, S.

An insight into the conformal flexibility and vibrational behavior of 2-nitroso-1-naphthol: A density functional theory approach
Spectroscopy Letters, (49): 294-303. 2016. 10.1080/00387010.2016.1145126

- Ragavendran, V.; Muthunatesan, S.
New insights into the conformal stability, influence of hydrogen bonding and vibrational analysis of 2,6-and 3,5-Dihydroxyacetophenone - A comparative study
Journal of Molecular Structure, (1125): 413-425. 2016. 10.1016/j.molstruc.2016.07.011
- Rahm, M.; Hoffmann, R.
Distinguishing Bonds
Journal of the American Chemical Society, (138): 3731-3744. 2016. 10.1021/jacs.5b12434
- Rahmanifar, E.; Yoosefian, M.; Karimi-Maleh, H.
Electronic properties and reactivity trend for defect functionalization of single-walled carbon nanotube with B, Al, Ga atoms
Synthetic Metals, (221): 242-246. 2016. 10.1016/j.synthmet.2016.09.017
- Rajaraman, D.; Sundararajan, G.; Rajkumar, R.; Bharanidharan, S.; Krishnasamy, K.
Synthesis, crystal structure investigation, DFT studies and DPPH radical scavenging activity of 1-(furan-2-ylmethyl)-2,4,5-triphenyl-1H-imidazole derivatives
Journal of Molecular Structure, (1108): 698-707. 2016. 10.1016/j.molstruc.2015.11.084
- Rajesh, P.; Gunasekaran, S.; GnanaSambandan, T.; Seshadri, S.
Experimental and theoretical study of ornidazole
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (153): 496-504. 2016.
10.1016/j.saa.2015.08.032
- Ramalakshmi, R.; Maheswari, K.; Sharmila, D.; Paul, A.; Roisnel, T.; Halet, J. F.; Ghosh, S.
Reactivity of cyclopentadienyl transition metal(II) complexes with borate ligands: structural characterization of the toluene-activated molybdenum complex Cp^{}Mo(CO)(2)(eta(3)-CH₂C₆H₅)*
Dalton Transactions, (45): 16317-16324. 2016. 10.1039/c6dt02641a
- Ramanathan, N.; Sankaran, K.; Sundararajan, K.
PCl₃-C₆H₆ heterodimers: evidence for P center dot center dot center dot pi phosphorus bonding at low temperatures
Physical Chemistry Chemical Physics, (18): 19350-19358. 2016. 10.1039/c6cp03825e
- Ramanathan, N.; Sundararajan, K.; Vidya, K.; Jemmis, E. D.
Non-covalent C-Cl center dot center dot center dot pi interaction in acetylene-carbon tetrachloride adducts: Matrix isolation infrared and ab initio computational studies
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (157): 69-78. 2016. 10.1016/j.saa.2015.12.016
- Ramasami, P.; Ford, T. A.
The structures and vibrational spectra of the methyl halide dimers. An ab initio study
Journal of Molecular Structure, (1126): 2-10. 2016. 10.1016/j.molstruc.2016.03.003
- Ramegowda, M.; Ranjitha, K. N.; Deepika, T. N.
Exploring excited state properties of 7-hydroxy and 7-methoxy 4-methycoumarin: a combined time-dependent density functional theory/effective fragment potential study
New Journal of Chemistry, (40): 2211-2219. 2016. 10.1039/c5nj02917a
- Rana, M.; Singla, N.; Chatterjee, A.; Shukla, A.; Chowdhury, P.
Investigation of nonlinear optical (NLO) properties by charge transfer contributions of amine functionalized tetraphenylethylene
Optical Materials, (62): 80-89. 2016. 10.1016/j.optmat.2016.09.043
- Rao, A. B. P.; Palepu, N. R.; Deb, D. K.; Uma, A.; Chiranjeevi, T.; Sarkar, B.; Kaminsky, W.; Rao, K. M.
Synthesis, structural, DFT studies and antibacterial evaluation of Cp^{} rhodium and Cp^{*} iridium complexes using hydrazide based dipyridyl ketone ligand*
Inorganica Chimica Acta, (443): 126-135. 2016. 10.1016/j.ica.2015.12.035
- Rao, A. B. P.; Uma, A.; Chiranjeevi, T.; Bethu, M. S.; Rao, J. V.; Deb, D. K.; Sarkar, B.; Kaminsky, W.; Kollipara, M. R.

The in vitro antitumor activity of oligonuclear polypyridyl rhodium and iridium complexes against cancer cells and human pathogens
Journal of Organometallic Chemistry, (824): 131-139. 2016. 10.1016/j.jorgchem.2016.10.018

Rao, C. E.; Barik, S. K.; Yuvaraj, K.; Bakthavachalam, K.; Roisnel, T.; Dorcet, V.; Halet, J. F.; Ghosh, S.
Reactivity of CS₂ - Syntheses and Structures of Transition-Metal Species with Dithioformate and Methanedithiolate Ligands
European Journal of Inorganic Chemistry: 4913-4920. 2016. 10.1002/ejic.201600823

Rao, J. L.; Bhanuprakash, K.
Push-pull effect on the geometrical, optical and charge transfer properties of disubstituted derivatives of mer-tris(4-hydroxy-1,5-naphthyridinato) aluminum (mer-AlND₃)
Open Chemistry, (14): 20-32. 2016. 10.1515/chem-2016-0001

Rao, N. Z.; Larkin, J. D.; Bock, C. W.
A comparison of the structure and bonding in the aliphatic boronic R-B(OH)(2) and borinic R-BH(OH) acids (R=H; NH₂, OH, and F): a computational investigation
Structural Chemistry, (27): 1081-1091. 2016. 10.1007/s11224-015-0730-5

Rao, S. S.; Gejji, S. P.
CO₂ Absorption Using Fluorine Functionalized Ionic Liquids: Interplay of Hydrogen and sigma-Hole Interactions
Journal of Physical Chemistry A, (120): 1243-1260. 2016. 10.1021/acs.jpca.5b12161

Rao, S. S.; Gejji, S. P.
Electronic Structure, NMR, Spin-Spin Coupling, and Noncovalent Interactions in Aromatic Amino Acid Based Ionic Liquids
Journal of Physical Chemistry A, (120): 5665-5684. 2016. 10.1021/acs.jpca.6b03985

Rao, S. S.; Lande, D. N.; Gejji, S. P.
Density functional theory investigations on binding and spectral features of complexes of ferrocenyl derivatives with cucurbit 7 uril
Journal of Molecular Liquids, (216): 298-308. 2016. 10.1016/j.molliq.2015.12.090

Rao, Y. B. S.; Prasad, M. V. S.; Sri, N. U.; Veeraiah, V.
Vibrational (FT-IR, FT-Raman) and UV-Visible spectroscopic studies, HOMO-LUMO, NBO, NLO and MEP analysis of Benzyl (imino (1H-pyrazol-1-yl) methyl) carbamate using DFT calculations
Journal of Molecular Structure, (1108): 567-582. 2016. 10.1016/j.molstruc.2015.12.008

Raugei, S.; Helm, M. L.; Hammes-Schiffer, S.; Appel, A. M.; O'Hagan, M.; Wiedner, E. S.; Bullock, R. M.
Experimental and Computational Mechanistic Studies Guiding the Rational Design of Molecular Electrocatalysts for Production and Oxidation of Hydrogen
Inorganic Chemistry, (55): 445-460. 2016. 10.1021/acs.inorgchem.5b02262

Raveendra, M.; Chandrasekhar, M.; Narasimharao, C.; Venkatramanna, L.; Kumar, K. S.; Reddy, K. D.
Elucidation of hydrogen bonding formation by a computational, FT-IR spectroscopic and theoretical study between benzyl alcohol and isomeric cresols
RSC Advances, (6): 27335-27348. 2016. 10.1039/c5ra26298d

Ravera, M.; Gabano, E.; Zanellato, I.; Fregonese, F.; Pelosi, G.; Platts, J. A.; Osella, D.
Antiproliferative activity of a series of cisplatin-based Pt(IV)-acetyl amido/carboxylato prodrugs
Dalton Transactions, (45): 5300-5309. 2016. 10.1039/c5dt04905a

Rawat, K. S.; Mahata, A.; Choudhuri, I.; Pathak, B.
Catalytic Hydrogenation of CO₂ by Manganese Complexes: Role of pi-Acceptor Ligands
Journal of Physical Chemistry C, (120): 16478-16488. 2016. 10.1021/acs.jpcc.6b05065

Rawat, K. S.; Mahata, A.; Choudhuri, I.; Pathak, B.
N-Heterocyclic Carbene-Based Mn Electrocatalyst for Two-Electron CO₂ Reduction over Proton Reduction

Journal of Physical Chemistry C, (120): 8821-8831. 2016. 10.1021/acs.jpcc.6b02209

Ray, A.; Panigrahi, S.; Bhattacharyya, D.

A Comparison of Four Different Conformations Adopted by Human Telomeric G-Quadruplex Using Computer Simulations

Biopolymers, (105): 83-99. 2016. 10.1002/bip.22751

Real, F.; Gomes, A. S. P.; Martinez, Y. O. G.; Ayed, T.; Galland, N.; Masella, M.; Vallet, V.

Structural, dynamical, and transport properties of the hydrated halides: How do At- bulk properties compare with those of the other halides, from F- to I-?

Journal of Chemical Physics, (144) 2016. 10.1063/1.4944613

Reddy, D. S.; Kutateladze, A. G.

Structure Revision of an Acorane Sesquiterpene Cordycepol A

Organic Letters, (18): 4860-4863. 2016. 10.1021/acs.orglett.6b02341

Reddy, G. N.; Giri, S.

Organic heterocyclic molecules become superalkalis

Physical Chemistry Chemical Physics, (18): 24356-24360. 2016. 10.1039/c6cp04430a

Reddy, V. P.; Mukherjee, S.; Mitra, I.; Misra, K.; Sengupta, P. S.; Linert, W.; Bose, J. C.; Ghosh, G. K.; Moi, S. C.

An experimental and theoretical approach on the kinetics and mechanism for the formation of a four-membered (S, S) chelated Pt(II) complex

RSC Advances, (6): 18288-18299. 2016. 10.1039/c5ra21161a

Rehman, H. U.; McKee, N. A.; McKee, M. L.

Saturn Systems

Journal of Computational Chemistry, (37): 194-209. 2016. 10.1002/jcc.23979

Reis, M. C.; Lopez, C. S.; Kraka, E.; Cremer, D.; Faza, O. N.

Rational Design in Catalysis: A Mechanistic Study of beta-Hydride Eliminations in Gold(I) and Gold(III) Complexes Based on Features of the Reaction Valley

Inorganic Chemistry, (55): 8636-8645. 2016. 10.1021/acs.inorgchem.6b01188

Reisi-Vanani, A.; Mehrdoust, S.

Effect of boron doping in sumanene frame toward hydrogen physisorption: A theoretical study

International Journal of Hydrogen Energy, (41): 15254-15265. 2016. 10.1016/j.ijhydene.2016.07.027

Rekha, T. N.; Rajkumar, B. J. M.

Nonlinear optical and charge transfer properties of tetracene adsorbed on silver: A DFT approach

Synthetic Metals, (215): 207-215. 2016. 10.1016/j.synthmet.2016.02.020

Rekha, T. N.; Rajkumar, B. J. M.

Spectroscopic and structural study of adsorption of benzene on silver using DFT

Journal of Computational Electronics, (15): 729-740. 2016. 10.1007/s10825-016-0841-2

Rekhroukh, F.; Estevez, L.; Bijani, C.; Miqueu, K.; Amgoune, A.; Bourissou, D.

Coordination-Insertion of Norbornene at Gold: A Mechanistic Study

Organometallics, (35): 995-1001. 2016. 10.1021/acs.organomet.6b00040

Rekhroukh, F.; Estevez, L.; Bijani, C.; Miqueu, K.; Amgoune, A.; Bourissou, D.

Experimental and Theoretical Evidence for an Agostic Interaction in a Gold(III) Complex

Angewandte Chemie-International Edition, (55): 3414-3418. 2016. 10.1002/anie.201511111

Rekhroukh, F.; Estevez, L.; Mallet-Ladeira, S.; Miqueu, K.; Amgoune, A.; Bourissou, D.

beta-Hydride Elimination at Low-Coordinate Gold(III) Centers

Journal of the American Chemical Society, (138): 11920-11929. 2016. 10.1021/jacs.6b07035

- Ren, F. D.; Cao, D. L.; Shi, W. J.; Gao, H. F.
A theoretical prediction of the relationships between the impact sensitivity and electrostatic potential in strained cyclic explosive and application to H-bonded complex of nitrocyclohydrocarbon
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2967-3
- Ren, L. K.; Yang, H. Q.; Hu, C. W.
Theoretical study of the catalytic oxidation mechanism of 5-hydroxymethylfurfural to 2,5-diformylfuran by PMo-containing Keggin heteropolyacid
Catalysis Science & Technology, (6): 3776-3787. 2016. 10.1039/c5cy01895a
- Reshetova, K. I.; Krauklis, I. V.; Litke, S. V.; Ershov, A. Y.; Chizhov, Y. V.
Spectroscopy and quantum-chemical calculations of nitro-bis-bipyridyl complexes of ruthenium(II) with 4-substituted pyridine ligands
Optics and Spectroscopy, (120): 566-574. 2016. 10.1134/s0030400x16040196
- Reveles, J. U.; Karle, N. N.; Baruah, T.; Zope, R. R.
Electronic and Structural Properties of C-60 and Sc3N@C-80 Supported on Graphene Nanoflakes
Journal of Physical Chemistry C, (120): 26083-26092. 2016. 10.1021/acs.jpcc.6b07405
- Reveles, J. U.; Saoud, K. M.; El-Shall, M. S.
Water inhibits CO oxidation on gold cations in the gas phase. Structures and binding energies of the sequential addition of CO, H₂O, O₂, and N₂ onto Au⁺
Physical Chemistry Chemical Physics, (18): 28606-28616. 2016. 10.1039/c6cp05431e
- Rezaeian, M.; Izadyar, M.
Theoretical investigation of the thermal decomposition of imidazolium ionic liquids with different halides ions
Journal of Molecular Liquids, (224): 460-465. 2016. 10.1016/j.molliq.2016.10.028
- Rezaei-Sameti, M.; Padervand, V.
A computational study of hydrogen cyanide interaction with the pristine and B, Ga, BGa-doped of (8,0) zigzag AlPNTs
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (86): 359-373. 2016. 10.1007/s10847-016-0668-2
- Ribblett, A. Q.; Poole, J. S.
A Laser Flash Photolysis Study of Azo-Compound Formation from Aryl Nitrenes at Room Temperature
Journal of Physical Chemistry A, (120): 4267-4276. 2016. 10.1021/acs.jpca.6b03025
- Richter, W. E.; Duarte, L. J.; Silva, A. F.; Bruns, R. E.
Review of Experimental GAP/T and Infrared Atomic Charges in Molecules
Journal of the Brazilian Chemical Society, (27): 979-991. 2016. 10.5935/0103-5053.20160105
- Rick, S. W.
A polarizable, charge transfer model of water using the drude oscillator
Journal of Computational Chemistry, (37): 2060-2066. 2016. 10.1002/jcc.24426
- Riddlestone, I. M.; McKay, D.; Gutmann, M. J.; Macgregor, S. A.; Mahon, M. F.; Sparkes, H. A.; Whittlesey, M. K.
Isolation of Ru(IPr)(2)(CO)H (+) (IPr=1,3-Bis(2,6-diisopropylphenyl)imidazol-2-ylidene) and Reactivity toward E-H (E = H, B) Bonds
Organometallics, (35): 1301-1312. 2016. 10.1021/acs.organomet.6b00173
- Rimac, H.; Debeljak, Z.; Sakic, D.; Weitner, T.; Gabricevic, M.; Vrcek, V.; Zorc, B.; Bojic, M.
Structural and electronic determinants of flavonoid binding to human serum albumin: an extensive ligand-based study
RSC Advances, (6): 75014-75022. 2016. 10.1039/c6ra17796d
- Rimsza, J. M.; Li, Y.; Pasquale, F.; Kelber, J.; Du, J. C.
Chemical bonding in carborane/aromatic co-polymers: a first-principles analysis of experimental photoemission spectra
Molecular Simulation, (42): 39-46. 2016. 10.1080/08927022.2015.1007055

- Rincon, D. A.; Cordeiro, M.; Mosquera, R. A.
On the effects of the basis set superposition error on the change of QTAIM charges in adduct formation. Application to complexes between morphine and cocaine and their main metabolites
RSC Advances, (6): 110642-110655. 2016. 10.1039/c6ra22736h
- Rios-Gutierrez, M.; Chafaa, F.; Nacereddine, A. K.; Djerourou, A.; Domingo, L. R.
A DFT study of 3+2 cycloaddition reactions of an azomethine imine with N-vinyl pyrrole and N-vinyl tetrahydroindole
Journal of Molecular Graphics & Modelling, (70): 296-304. 2016. 10.1016/j.jmgm.2016.10.009
- Robinson, R.; Shaw, M. F.; Stranger, R.; Yates, B. F.
Theoretical study of the mechanism for the sequential N-O and N-N bond cleavage within N₂O adducts of N-heterocyclic carbenes by a vanadium(III) complex
Dalton Transactions, (45): 1047-1054. 2016. 10.1039/c5dt03600c
- Roca, S.; Vikic-Topic, D.; Plavec, J.; Sket, P.; Mihalic, Z.; Matkovic-Calogovic, D.; Popovic, Z.
Structural diversity of the Ag coordination sphere in complexes of silver(I) nitrate with 3-halopyridine. Characterization of the complexes in solution and in the solid state
Polyhedron, (109): 166-175. 2016. 10.1016/j.poly.2016.01.047
- Rodrigues, D. N. S.; Olivato, P. R.; Rodrigues, A.; Dal Colle, M.
Conformational analysis and electronic interactions of some 2-ethylsulfinyl-(4'-substituted)-phenylacetates
Journal of Molecular Structure, (1108): 245-256. 2016. 10.1016/j.molstruc.2015.12.022
- Rodrigues, D. N. S.; Olivato, P. R.; Zukerman-Schpector, J.; Tiekink, E. R. T.
Spectroscopic and theoretical studies of some 4'-substituted-phenyl 2-(ethanesulfonyl)acetates. Structure of 4'-nitrophenyl 2-(ethanesulfonyl) acetate
Zeitschrift Fur Kristallographie-Crystalline Materials, (231): 23-34. 2016. 10.1515/zkri-2015-1879
- Rodriguez-Castillo, M.; Lugo-Preciado, G.; Laurencin, D.; Tielen, F.; van der Lee, A.; Clement, S.; Guari, Y.; Lopez-de-Luzuriaga, J. M.; Monge, M.; Remacle, F.; Richeter, S.
Experimental and Theoretical Study of the Reactivity of Gold Nanoparticles Towards Benzimidazole-2-ylidene Ligands
Chemistry-a European Journal, (22): 10446-10458. 2016. 10.1002/chem.201601253
- Roffey, A.; Hollingsworth, N.; Islam, H. U.; Mercy, M.; Sankar, G.; Catlow, C. R. A.; Hogarth, G.; de Leeuw, N. H.
Phase control during the synthesis of nickel sulfide nanoparticles from dithiocarbamate precursors
Nanoscale, (8): 11067-11075. 2016. 10.1039/c6nr00053c
- Rogers, I. L.; Naidoo, K. J.
Multidimensional Reaction Dynamics Reveal How the Enzyme TcTS Suppresses Competing Side Reactions and Their Side Products
ACS Catalysis, (6): 6384-6392. 2016. 10.1021/acscatal.6b01522
- Rokob, T. A.
Pathways for Arene Oxidation in Non-Heme Diiron Enzymes: Lessons from Computational Studies on Benzoyl Coenzyme A Epoxidase
Journal of the American Chemical Society, (138): 14623-14638. 2016. 10.1021/jacs.6b06987
- Romani, D.; Tsuchiya, S.; Yotsu-Yamashita, M.; Brandan, S. A.
Spectroscopic and structural investigation on intermediates species structurally associated to the tricyclic bisguanidine compound and to the toxic agent, saxitoxin
Journal of Molecular Structure, (1119): 25-38. 2016. 10.1016/j.molstruc.2016.04.039
- Romero-Fernandez, M. P.; Avalos, M.; Babiano, R.; Cintas, P.; Jimenez, J. L.; Palacios, J. C.
A further look at pi-delocalization and hydrogen bonding in 2-arylmalondialdehydes
Tetrahedron, (72): 95-104. 2016. 10.1016/j.tet.2015.11.006
- Roohi, H.; Ghauri, K.

Influence of various anions and cations on electrochemical and physicochemical properties of the nanostructured Tunable Aryl Alkyl Ionic Liquids (TAAILs): A DFT M06-2X study
Thermochimica Acta, (639): 20-40. 2016. 10.1016/j.tca.2016.07.003

Roohi, H.; Maleki, L.
Effects of C1-3-doping on electronic and structural properties of Stone-Wales defective boron nitride nanotubes as well as their NO gas sensitivity
RSC Advances, (6): 11353-11369. 2016. 10.1039/c5ra20920j

Roohi, H.; Nokhostin, R.; Mohamadnia, M.
Photoswitching in nanostructured benzofuro 3,2-b pyridin-9-ol and benzothio 3,2-b pyridin-9-ol compounds as red-and yellow-light-emitting molecules: A TD-DFT approach
Dyes and Pigments, (134): 106-117. 2016. 10.1016/j.dyepig.2016.07.004

Rosenberg, R. E.
Microsolvation of Fluoromethane
Journal of Physical Chemistry A, (120): 7519-7528. 2016. 10.1021/acs.jpca.6b07063

Rosener, T.; Bienemann, O.; Sigl, K.; Schopp, N.; Schnitter, F.; Florke, U.; Hoffmann, A.; Doring, A.; Kuckling, D.; Herres-Pawlisch, S.
A Comprehensive Study of Copper Guanidine Quinoline Complexes: Predicting the Activity of Catalysts in ATRP with DFT
Chemistry-a European Journal, (22): 13550-13562. 2016. 10.1002/chem.201602223

Rosenow, P.; Jakob, P.; Tonner, R.
Electron-Vibron Coupling at Metal-Organic Interfaces from Theory and Experiment
Journal of Physical Chemistry Letters, (7): 1422-1427. 2016. 10.1021/acs.jpclett.6b00299

Rosokha, S. V.; Lukacs, E.; Ritzert, J. T.; Wasilewski, A.
Mechanism and Thermodynamics of Reductive Cleavage of Carbon-Halogen Bonds in the Polybrominated Aliphatic Electrophiles
Journal of Physical Chemistry A, (120): 1706-1715. 2016. 10.1021/acs.jpca.5b11410

Rosselin, M.; Tuccio, B.; Perio, P.; Villamena, F. A.; Fabre, P. L.; Durand, G.
Electrochemical and Spin-Trapping Properties of para-substituted alpha-Phenyl-N-tert-butyl Nitrones
Electrochimica Acta, (193): 231-239. 2016. 10.1016/j.electacta.2016.02.038

Roy, D. K.; Borthakur, R.; Prakash, R.; Bhattacharya, S.; Jagan, R.; Ghosh, S.
Hypoelectronic 8-11-Vertex Irida- and Rhodaboranes
Inorganic Chemistry, (55): 4764-4770. 2016. 10.1021/acs.inorgchem.6b00076

Roy, D. K.; Yuvaraj, K.; Jagan, R.; Ghosh, S.
Chemistry of Rh-N,S heterocyclic carbene complexes
Journal of Organometallic Chemistry, (811): 8-13. 2016. 10.1016/j.jorganchem.2016.03.012

Roy, S.; Bhattacharyya, A.; Purkait, S.; Bauza, A.; Frontera, A.; Chattopadhyay, S.
A combined experimental and computational study on supramolecular assemblies in hetero-tetrานuclear nickel(II)-cadmium(II) complexes with N2O4-donor compartmental Schiff bases
Dalton Transactions, (45): 15048-15059. 2016. 10.1039/c6dt02587k

Roy, S.; Kastner, J.
Synergistic Substrate and Oxygen Activation in Salicylate Dioxygenase Revealed by QM/MM Simulations
Angewandte Chemie-International Edition, (55): 1168-1172. 2016. 10.1002/anie.201506363

Roy, S. K.; Jian, T.; Lopez, G. V.; Li, W. L.; Su, J.; Bross, D. H.; Peterson, K. A.; Wang, L. S.; Li, J.
A combined photoelectron spectroscopy and relativistic ab initio studies of the electronic structures of UFO and UFO
Journal of Chemical Physics, (144) 2016. 10.1063/1.4942188

Rozada, T. D.; Pontes, R. M.; Rittner, R.; Basso, E. A.

Stereoelectronic effects of the glycosidic linkage on the conformational preference of D-sucrose
RSC Advances, (6): 112806-112812. 2016. 10.1039/c6ra24413k

Roztoczynska, A.; Kozlowska, J.; Lipkowski, P.; Bartkowiak, W.
Hydrogen bonding inside and outside carbon nanotubes: HF dimer as a case study
Physical Chemistry Chemical Physics, (18): 2417-2427. 2016. 10.1039/c5cp04153h

Ruccolo, S.; Sattler, W.; Rong, Y.; Parkin, G.
Modulation of Zn-C Bond Lengths Induced by Ligand Architecture in Zinc Carbatrane Compounds
Journal of the American Chemical Society, (138): 14542-14545. 2016. 10.1021/jacs.6b09250

Ruiz, P.; Castro, M.; Lopez, S.; Zapata, A.; Quijano, J.; Notario, R.
Computational study of the thermal decomposition of 2-methylbutyraldehyde and 2-pentanone through retro-ene reactions
Structural Chemistry, (27): 1373-1381. 2016. 10.1007/s11224-016-0757-2

Russo, M. G.; Sancho, M. I.; Silva, L. M. A.; Baldoni, H. A.; Venancio, T.; Ellena, J.; Narda, G. E.
Looking for the interactions between omeprazole and amoxicillin in a disordered phase. An experimental and theoretical study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (156): 70-77. 2016. 10.1016/j.saa.2015.11.021

Saadat, K.; Tavakol, H.
Study of noncovalent interactions of end-capped sulfur-doped carbon nanotubes using DFT, QTAIM, NBO and NCI calculations
Structural Chemistry, (27): 739-751. 2016. 10.1007/s11224-015-0616-6

Saberinasab, M.; Salehzadeh, S.; Maghsoud, Y.; Bayat, M.
The significant effect of electron donating and electron withdrawing substituents on nature and strength of an intermolecular Se center dot center dot center dot pi interaction. A theoretical study
Computational and Theoretical Chemistry, (1078): 9-15. 2016. 10.1016/j.comptc.2015.12.009

Saberinasab, M.; Salehzadeh, S.; Solimannejad, M.
The effect of a strong cation center dot center dot center dot pi interaction on a weak selenium center dot center dot center dot pi interaction: A theoretical study
Computational and Theoretical Chemistry, (1092): 41-46. 2016. 10.1016/j.comptc.2016.07.027

Sabet-Sarvestani, H.; Eshghi, H.; Izadyar, M.; Bakavoli, M.
NCI concept as a powerful tool to investigate the origin of Diels-Alder reaction accelerating inside the self-assembled softball nanoreactor
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (85): 237-246. 2016. 10.1007/s10847-016-0623-2

Sabet-Sarvestani, H.; Eshghi, H.; Izadyar, M.; Noroozi-Shad, N.; Bakavoli, M.; Ziaeef, F.
Borohydride salts as high efficiency reducing reagents for carbon dioxide transformation to methanol: Theoretical approach
International Journal of Hydrogen Energy, (41): 11131-11140. 2016. 10.1016/j.ijhydene.2016.05.050

Sabounchei, S. J.; Ahmadianpoor, M.; Yousefi, A.; Hashemi, A.; Bayat, M.; Sedghi, A.; Bagherjeri, F. A.; Gable, R. W.
New Pd(II) complexes of sulfur ylides; synthesis, X-ray characterization, a theoretical study and catalytic activity toward the Mizoroki-Heck reaction
RSC Advances, (6): 28308-28315. 2016. 10.1039/c6ra01390b

Sabounchei, S. J.; Yousefi, A.; Ahmadianpoor, M.; Hashemi, A.; Bayat, M.; Sedghi, A.; Bagherjeri, F. A.; Gable, R. W.
A new Pd(II) complex of a sulfur ylide; Synthesis, X-ray characterization, theoretical study and catalytic activity toward the Suzuki-Miyaura reaction
Polyhedron, (117): 273-282. 2016. 10.1016/j.poly.2016.05.046

Sabounchei, S. J.; Zamanian, M.; Pourshahbaz, M.; Bayat, M.; Karamian, R.; Asadbegy, M.

Synthesis, characterisation and theoretical and antibacterial studies of Hg(II), Cd(II) and Ag(I) complexes with a new monodentate phosphorus ylide

Journal of Chemical Research: 130-136. 2016. 10.3184/174751916x14537279217786

Sadhu, B.; Sundararajan, M.; Bandyopadhyay, T.

Efficient Separation of Europium Over Americium Using Cucurbit- 5 -uril Supramolecule: A Relativistic DFT Based Investigation

Inorganic Chemistry, (55): 598-609. 2016. 10.1021/acs.inorgchem.5b01627

Saeed, A.; Arshad, M. I.; Bolte, M.; Fantoni, A. C.; Espinoza, Z. Y. D.; Erben, M. F.

On the roles of close shell interactions in the structure of acyl-substituted hydrazones: An experimental and theoretical approach

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (157): 138-145. 2016.

10.1016/j.saa.2015.12.026

Saez, D. A.; Vogt-Geisse, S.; Inostroza-Rivera, R.; Kubar, T.; Elstner, M.; Toro-Labbe, A.; Vohringer-Martinez, E.

The effect of the environment on the methyl transfer reaction mechanism between trimethylsulfonium and phenolate

Physical Chemistry Chemical Physics, (18): 24033-24042. 2016. 10.1039/c6cp02821g

Safi, Z. S.

A theoretical study on the structure of thiazolidine-2,4-dione and its 5-substituted derivatives in the gas phase.

Implications for the thiazolidine-2,4-dione -water complex

Arabian Journal of Chemistry, (9): 616-625. 2016. 10.1016/j.arabjc.2015.03.016

Saha, P.; Rahane, A. B.; Kumar, V.; Sukumar, N.

Analysis of the electron density features of small boron clusters and the effects of doping with C, P, Al, Si, and Zn:

Magic B₇P and B₈Si clusters

Physica Scripta, (91) 2016. 10.1088/0031-8949/91/5/053005

Saha, R.; Pan, S.; Mandal, S.; Orozco, M.; Merino, G.; Chattaraj, P. K.

Noble gas supported B-3(+) cluster: formation of strong covalent noble gas-boron bonds

RSC Advances, (6): 78611-78620. 2016. 10.1039/c6ra16188j

Saikia, E.; Borpuzari, M. P.; Chetia, B.; Kar, R.

Experimental and theoretical study of urea and thiourea based new colorimetric chemosensor for fluoride and acetate ions

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (152): 101-108. 2016.

10.1016/j.saa.2015.07.065

Saleh, T. S.; Hussein, M. A.; Osman, O. I.; Alamry, K. A.; Mekky, A. E. M.; Asiri, A. M.; El-Daly, S. A.

Photophysical Behavior and Computational Investigation of Novel 1,4-Bis(2-(2-Phenylpyrimido 1,2-a Benzimidazol-4-Yl)Phenoxy)Butan (BPPB) Macromolecule

Journal of Fluorescence, (26): 1895-1904. 2016. 10.1007/s10895-016-1884-2

Salehi, S.; Saljooghi, A. S.; Izadyar, M.

A theoretical study on the electronic structures and equilibrium constants evaluation of Deferasirox iron complexes

Computational Biology and Chemistry, (64): 99-106. 2016. 10.1016/j.combiolchem.2016.05.010

Samanta, P. N.; Das, K. K.

Prediction of binding modes and affinities of 4-substituted-2,3,5,6-tetrafluorobenzenesulfonamide inhibitors to the carbonic anhydrase receptor by docking and ONIOM calculations

Journal of Molecular Graphics & Modelling, (63): 38-48. 2016. 10.1016/j.jmgm.2015.11.010

Samiee, S.; Mandavifar, Z.; Azadmanesh, A.; Jalilian, F.; Rahbari, M. N.

Different coordination modes of bifunctionalized ylides in complexation with group 12 metals via computational approach

Journal of Molecular Liquids, (219): 579-591. 2016. 10.1016/j.molliq.2016.03.033

Samsonowicz, M.; Kowczyk-Sadowy, M.; Piekut, J.; Regulska, E.; Lewandowski, W.
Spectroscopic characteristic (FT-IR, FT-Raman, UV, H-1 and C-13 NMR), theoretical calculations and biological activity of alkali metal homovanillates
Journal of Molecular Structure, (1109): 1-12. 2016. 10.1016/j.molstruc.2015.12.062

Samzadeh-Kermani, A.
One-pot synthesis of heterocyclic compounds containing highly polarized double bond
Monatshefte fur Chemie, (147): 761-765. 2016. 10.1007/s00706-015-1529-1

Sanchez-Marquez, J.
Introducing new reactivity descriptors: "Bond reactivity indices." Comparison of the new definitions and atomic reactivity indices
Journal of Chemical Physics, (145) 2016. 10.1063/1.4967293

Sanchez-Sanz, G.; Trujillo, C.; Alkorta, I.
Structure, binding energy and chiral discrimination in oxathirane homodimers
Computational and Theoretical Chemistry, (1090): 171-179. 2016. 10.1016/j.comptc.2016.06.020

Sanchez-Sanz, G.; Trujillo, C.; Alkorta, I.; Elguero, J.
Aromatic changes in isoelectronic derivatives of phenalenyl radicals by central carbon replacement
Tetrahedron, (72): 4690-4699. 2016. 10.1016/j.tet.2016.06.050

Sanchez-Sanz, G.; Trujillo, C.; Alkorta, I.; Elguero, J.
Competition between intramolecular hydrogen and pnictogen bonds in protonated systems
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1895-8

Sanchez-Sanz, G.; Trujillo, C.; Alkorta, I.; Elguero, J.
Modulating intramolecular P center dot center dot center dot N pnictogen interactions
Physical Chemistry Chemical Physics, (18): 9148-9160. 2016. 10.1039/c6cp00227g

Sancinetto, L.; Tidei, C.; Bagnoli, L.; Marini, F.; Lippolis, V.; Arca, M.; Lenardao, E. J.; Santi, C.
Synthesis of Thiol Esters Using PhS_nZnBr as Sulfenylation Agent: A DFT-Guided Optimization of Reaction Conditions
European Journal of Organic Chemistry: 2999-3005. 2016. 10.1002/ejoc.201600366

Sang, Y. T.; Fu, A. P.; Li, H.; Zhang, J. T.; Li, Z. C.; Li, H. L.; Zhao, X. S.; Guo, P. Z.
Experimental and theoretical studies on the effect of functional groups on carbon nanotubes to its oxygen reduction reaction activity
Colloids and Surfaces a-Physicochemical and Engineering Aspects, (506): 476-484. 2016.
10.1016/j.colsurfa.2016.07.008

Sangeetha, K.; Prasad, L. G.; Mathammal, R.
Crystal growth, vibrational, optical, thermal and theoretical studies of a nonlinear optical material: 2-Methyl 3,5-dinitrobenzoic acid
Physica B-Condensed Matter, (501): 5-17. 2016. 10.1016/j.physb.2016.08.006

Sangeetha, M.; Mathammal, R.
A complete synergy on the experimental and theoretical study of the pyridine derivatives-2-Hydroxy-5-Nitropyridine and 2-Chloro-5-Nitropyridine
Journal of Molecular Structure, (1117): 121-134. 2016. 10.1016/j.molstruc.2016.03.070

Sangilipandi, S.; Sutradhar, D.; Bhattacharjee, K.; Kaminsky, W.; Joshi, S. R.; Chandra, A. K.; Rao, K. M.
Synthesis, structure, antibacterial studies and DFT calculations of arene ruthenium, Cp^{}Rh, Cp^{*}Ir and tricarbonylrhenium metal complexes containing 2-chloro-3-(3-(2-pyridyl)pyrazolyl)quinoxaline ligand*
Inorganica Chimica Acta, (441): 95-108. 2016. 10.1016/j.ica.2015.11.012

Sangilipandi, S.; Sutradhar, D.; Kaminsky, W.; Chandra, A. K.; Rao, K. M.
Synthesis, molecular structure and DFT studies of tricarbonylrhenium(I) complexes containing nitrogen based bis, Iris, tetrakis-(di-2-pyridylaminomethyl)benzene ligands

Journal of Molecular Structure, (1115): 8-16. 2016. 10.1016/j.molstruc.2016.02.078

Sanina, N. A.; Shmatko, N. Y.; Korchagin, D. V.; Shilov, G. V.; Terent'ev, A. A.; Stupina, T. S.; Balakina, A. A.; Komleva, N. V.; Ovanesyan, N. S.; Kulikov, A. V.; Aldoshin, S. M.

A new member of the cationic dinitrosyl iron complexes family incorporating N-ethylthiourea is effective against human HeLa and MCF-7 tumor cell lines

Journal of Coordination Chemistry, (69): 812-825. 2016. 10.1080/00958972.2016.1142536

SanthiBhushan, B.; Khan, M. S.; Srivastava, A.; Khan, M. S.

First Principle Analysis of (10-Boranylanthracene-9-yl)borane-Based Molecular Single-Electron Transistor for High-Speed Low-Power Electronics

IEEE Transactions on Electron Devices, (63): 1232-1238. 2016. 10.1109/ted.2016.2518713

Santiago, C. B.; Milo, A.; Sigman, M. S.

Developing a Modern Approach To Account for Steric Effects in Hammett-Type Correlations
Journal of the American Chemical Society, (138): 13424-13430. 2016. 10.1021/jacs.6b08799

Sanyal, R.; Zhang, X. P.; Chakraborty, P.; Mautner, F. A.; Zhao, C. Y.; Das, D.

Role of para-substitution in controlling phosphatase activity of dinuclear Ni-II complexes of Mannich-base ligands: experimental and DFT studies

RSC Advances, (6): 73534-73546. 2016. 10.1039/c6ra08705a

Sarada, K.; Vijisha, K. R.; Muraleedharan, K.

Exploration of the thermal decomposition of oxalates of copper and silver by experimental and computational methods

Journal of Analytical and Applied Pyrolysis, (120): 207-214. 2016. 10.1016/j.jaat.2016.05.007

Sarhadinia, S.; Ebrahimi, A.

H-bond and dipole-dipole interactions between water and -COO- functional group in methyl benzoate derivatives: Substituent and heteroatom effects

Journal of Molecular Graphics & Modelling, (70): 7-13. 2016. 10.1016/j.jmgm.2016.09.003

Sarioglu, A. O.; Ceylan, U.; Yalcin, S. P.; Sonmez, M.; Ceyhan, G.; Aygun, M.

Synthesis of a new ONNO donor tetradeятate schiff base ligand and binuclear Cu(II) complex: Quantum chemical, spectroscopic and photoluminescence investigations

Journal of Luminescence, (176): 193-201. 2016. 10.1016/j.jlumin.2016.03.021

Sarkar, S.; Pavan, M. S.; Cherukuvada, S.; Row, T. N. G.

Acetazolamide polymorphism: a case of hybridization induced polymorphism?

Chemical Communications, (52): 5820-5823. 2016. 10.1039/c6cc01612j

Sarma, K.; Devi, N.; Sutradhar, D.; Sarma, B.; Chandra, A. K.; Barman, P.

Synthesis of a novel six membered CNS palladacycle; TD-DFT study and catalytic activity towards microwave-assisted selective oxidation of terminal olefin to aldehyde

Journal of Organometallic Chemistry, (822): 20-28. 2016. 10.1016/j.jorgchem.2016.08.006

Sarosi, M. B.; Hey-Hawkins, E.

RHODIUM(I) COMPLEXES OF BISPHOSPHONITOCARBABORANE(12)S: A COMPUTATIONAL STUDY
Studia Universitatis Babes-Bolyai Chemia, (61): 39-44. 2016.

Sas, E. B.; Kurt, M.; Can, M.; Horzum, N.; Atac, A.

Spectroscopic studies on 9H-carbazole-9-(4-phenyl) boronic acid pinacol ester by DFT method
Journal of Molecular Structure, (1118): 124-138. 2016. 10.1016/j.molstruc.2016.03.064

Sasi, B. S. A.; Bright, K. C.; James, C.

Vibrational spectral characterization, NLO studies and charge transfer analysis of the organometallic material L-Alanine cadmium chloride

Journal of Molecular Structure, (1103): 286-294. 2016. 10.1016/j.molstruc.2015.08.052

- Saska, J.; Lewis, W.; Paton, R. S.; Denton, R. M.
Synthesis of malhamensilipin A exploiting iterative epoxidation/chlorination: experimental and computational analysis of epoxide-derived chloronium ions
Chemical Science, (7): 7040-7049. 2016. 10.1039/c6sc03012b
- Sato, H.; Miyada, M.; Yamamoto, S.; Reddy, K. R.; Ozaki, Y.
C-H center dot center dot center dot O (ether) hydrogen bonding along the (110) direction in polyglycolic acid studied by infrared spectroscopy, wide-angle X-ray diffraction, quantum chemical calculations and natural bond orbital calculations
RSC Advances, (6): 16817-16823. 2016. 10.1039/c5ra19900j
- Saura, P.; Masgrau, L.; Heydeck, D.; Kuhn, H.; Lluch, J. M.; Gonzalez-Lafont, A.
Is Regioselectivity in the Enzyme-Catalyzed Hydroperoxidation of Arachidonic Acid Necessarily Determined by Hydrogen Abstraction? The Case of Rabbit Leu597Ala/Ile663Ala ALOX15 Mutant
Chemphyschem, (17): 3321-3332. 2016. 10.1002/cphc.201600534
- Savithiri, S.; Doss, M. A.; Rajarajan, G.; Thanikachalam, V.
Molecular structure, vibrational spectral assignments (FT-IR and FT-Raman), UV-Vis, NMR, NBO, HOMO-LUMO and NLO properties of 3t-penty1-2r,6c-diphenylpiperidin-4-one picrate based on DFT calculations
Journal of Molecular Structure, (1105): 225-237. 2016. 10.1016/j.molstruc.2015.10.063
- Sazonov, P. K.; Gloriozov, I. P.; Oprunenko, Y. F.; Beletskaya, I. P.
1,2-Shift of Element-Centered Groups (RnE) in Carbenoid Anions $RnECF_2CFCl$ (-) and its Relevance for Nucleophilic Vinylic Substitution: a DFT Study
Chemistryselect, (1): 3384-3396. 2016. 10.1002/slct.201600649
- Scheiner, S.
Assessment of the Presence and Strength of H-Bonds by Means of Corrected NMR
Molecules, (21) 2016. 10.3390/molecules21111426
- Scheiner, S.
Highly Selective Halide Receptors Based on Chalcogen, Pnicogen, and Tetrel Bonds
Chemistry-a European Journal, (22): 18850-18858. 2016. 10.1002/chem.201603891
- Schipper, D. E.; Ihklef, D.; Khalal, S.; Saillard, J. Y.; Whitmire, K. H.
New Main-Group-Element-Rich nido-Octahedral Cluster System: Synthesis and Characterization of $Et_4N Fe\{2(CO)(6)(mu(3)-As)\{mu(3)-EFe(CO)(4)\}(2)$
Inorganic Chemistry, (55): 6679-6684. 2016. 10.1021/acs.inorgchem.6b00921
- Schmidt, A.; Batsyts, S.; Smeyanov, A.; Freese, T.; Hubner, E. G.; Nieger, M.
Dipolar Bent and Linear Acetylenes Substituted by Cationic Quinolinium and Anionic Benzoates. Formation of Mesomeric Betaines
Journal of Organic Chemistry, (81): 4202-4209. 2016. 10.1021/acs.joc.6b00561
- Schnee, G.; Specklin, D.; Djukic, J. P.; Dagorne, S.
Deprotonation of Al_2Me_6 by Sterically Bulky NHCs: Scope, Rationale through DFT Studies, and Application in the Methylenation of Carbonyl Substrates
Organometallics, (35): 1726-1734. 2016. 10.1021/acs.organomet.6b00159
- Schneider, W. B.; Bistoni, G.; Sparta, M.; Saitow, M.; Riplinger, C.; Auer, A. A.; Neese, F.
Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework
Journal of Chemical Theory and Computation, (12): 4778-4792. 2016. 10.1021/acs.jctc.6b00523
- Schoeller, W. W.; Frey, G. D.
Oxidative Addition of pi-Bonds and sigma-Bonds to an $Al(I)$ Center: The Second-Order Carbene Property of the $AlNacNac$ Compound
Inorganic Chemistry, (55): 10947-10954. 2016. 10.1021/acs.inorgchem.6b01488

Schrappers, P.; Mebs, S.; Goetzl, S.; Hennig, S. E.; Dau, H.; Dobbek, H.; Haumann, M.
Axial Ligation and Redox Changes at the Cobalt Ion in Cobalamin Bound to Corrinoid Iron-Sulfur Protein (CoFeSP) or in Solution Characterized by XAS and DFT
PLoS One, (11) 2016. 10.1371/journal.pone.0158681

Schutz, M.; Bouchet, A.; Chiavarino, B.; Crestoni, M. E.; Fornarini, S.; Dopfer, O.
Effects of Aromatic Fluorine Substitution on Protonated Neurotransmitters: The Case of 2-Phenylethylamine
Chemistry-a European Journal, (22): 8124-8136. 2016. 10.1002/chem.201600798

Schutz, M.; Bouchet, A.; Dopfer, O.
Infrared spectrum of the cold ortho-fluorinated protonated neurotransmitter 2-phenylethylamine: competition between NH+center dot center dot center dot pi and NH+center dot center dot center dot F interactions
Physical Chemistry Chemical Physics, (18): 26980-26989. 2016. 10.1039/c6cp05915e

Schweizer, J. I.; Meyer, L.; Nadj, A.; Diefenbach, M.; Holthausen, M. C.
Unraveling the Amine-Induced Disproportionation Reaction of Perchlorinated Silanes-A DFT Study
Chemistry-a European Journal, (22): 14328-14335. 2016. 10.1002/chem.201602724

Scuderi, D.; Bodo, E.; Chiavarino, B.; Fornarini, S.; Crestoni, M. E.
Amino Acid Oxidation: A Combined Study of Cysteine Oxo Forms by IRMPD Spectroscopy and Simulations
Chemistry-a European Journal, (22): 17239-17250. 2016. 10.1002/chem.201603298

Sebastian, S. H. R.; Al-Alshaikh, M. A.; El-Emam, A. A.; Panicker, C. Y.; Zitko, J.; Dolezal, M.; VanAlsenoy, C.
Spectroscopic, quantum chemical studies, Fukui functions, in vitro antiviral activity and molecular docking of 5-chloro-N-(3-nitrophenyl) pyrazine-2-carboxamide
Journal of Molecular Structure, (1119): 188-199. 2016. 10.1016/j.molstruc.2016.04.088

Sebesta, F.; Burda, J. V.
Reduction Process of Tetraplatin in the Presence of Deoxyguanosine Monophosphate (dGMP): A Computational DFT Study
Chemistry-a European Journal, (22): 1037-1047. 2016. 10.1002/chem.201503555

Sedlak, R.; Stasyuk, O. A.; Guerra, C. F.; Rezac, J.; Ruzicka, A.; Hobza, P.
New Insight into the Nature of Bonding in the Dimers of Lappert's Stannylene and Its Ge Analogs: A Quantum Mechanical Study
Journal of Chemical Theory and Computation, (12): 1696-1704. 2016. 10.1021/acs.jctc.6b00065

Segala, M.; Schneider, F. S. S.; Caramori, G. F.; Parreira, R. L. T.
Evaluation of Electron Donation as a Mechanism for the Stabilisation of Chalcogenate-Protected Gold Nanoclusters
Chemphyschem, (17): 3102-3111. 2016. 10.1002/cphc.201600552

Seguin, T. J.; Wheeler, S. E.
Electrostatic Basis for Enantioselective Bronsted-Acid-Catalyzed Asymmetric Ring Openings of meso-Epoxides
ACS Catalysis, (6): 2681-2688. 2016. 10.1021/acscatal.6b00538

Selvakumar, S.; Boobalan, M. S.; Babu, S. A.; Ramalingam, S.; Rajesh, A. L.
Crystal growth and DFT insight on sodium para-nitrophenolate para-nitrophenol dihydrate single crystal for NLO applications
Journal of Molecular Structure, (1125): 1-11. 2016. 10.1016/j.molstruc.2016.05.104

Semenov, S. G.; Bedrina, M. E.; Egorov, N. V.; Titov, A. V.
Quantum-chemical study of lutetium, ytterbium, and gadolinium phthalocyaninates P_xLnCl_y
Russian Journal of General Chemistry, (86): 1095-1101. 2016. 10.1134/s1070363216050194

Semenov, S. G.; Bedrina, M. E.; Titov, A. V.
Quantum-chemical study of ytterbium fluorides and of complex F₂YbF₂CeF₂
Russian Journal of General Chemistry, (86): 1215-1220. 2016. 10.1134/s1070363216060013

- Semire, B.; Oyebamiji, A.; Odunola, O. A.
Design of (2Z)-2-cyano-2- 2- (E)-2- 5- (E)-2-(4-dimethylaminophenyl)vinyl -2-thien yl vinyl pyran-4-ylidene acetic acid derivatives as D-pi-A dye sensitizers in molecular photovoltaics: a density functional theory approach
Research on Chemical Intermediates, (42): 4605-4619. 2016. 10.1007/s11164-015-2303-z
- Sen, B.; Barim, E.; Kirilmis, C.; Aygun, M.
Synthesis, structural characterization, and DFT calculations of 3-buthyl-4-(3-methyl-3-mesitylcyclobut-1-yl)-1,3-thiazole-2(3H)-thione
Crystallography Reports, (61): 243-248. 2016. 10.1134/s1063774516020188
- Sengupta, A.; Ali, S. M.; Shenoy, K. T.
Understanding the complexation of the Eu³⁺ ion with TODGA, CMPO, TOPO and DMDBTDMA: Extraction, luminescence and theoretical investigation
Polyhedron, (117): 612-622. 2016. 10.1016/j.poly.2016.06.037
- Sengupta, A.; Jayabun, S.; Boda, A.; Ali, S. M.
An amide functionalized task specific carbon nanotube for the sorption of tetra and hexa valent actinides: experimental and theoretical insight
RSC Advances, (6): 39553-39562. 2016. 10.1039/c6ra07986e
- Sengupta, M.; Bag, A.; Das, S.; Shukla, A.; Konathala, L. N. S.; Naidu, C. A.; Bordoloi, A.
Reaction and Mechanistic Studies of Heterogeneous Hydroamination over Support-Stabilized Gold Nanoparticles
Chemcatchem, (8): 3121-3130. 2016. 10.1002/cctc.201600762
- Seo, D.; Park, K. W.; Kim, J.; Hong, J.; Kwak, K.
DFT computational investigation of tuning the electron donating ability in metal-free organic dyes featuring a thiénylthynyl spacer for dye sensitized solar cells
Computational and Theoretical Chemistry, (1081): 30-37. 2016. 10.1016/j.comptc.2016.02.009
- Seridi, L.; Boufelfel, A.; Soltani, S.
Structural, electronic and QTAIM analysis of host-guest interaction of Warfarin with beta-cyclodextrin and calix 4 arene
Journal of Molecular Liquids, (221): 885-895. 2016. 10.1016/j.molliq.2016.06.071
- Seridi, S.; Dinar, K.; Seridi, A.; Berredjem, M.; Kadri, M.
Charge transfer complexes of 4-isopropyl-2-benzyl-1,2,5-thiadiazolidin-3-one1,1-dioxide with DDQ and TCNE: experimental and DFT studies
New Journal of Chemistry, (40): 4781-4792. 2016. 10.1039/c5nj03017j
- Serobatse, K. R. N.; Kabanda, M. M.
Antioxidant and antimalarial properties of butein and homobutein based on their ability to chelate iron (II and III) cations: a DFT study in vacuo and in solution
European Food Research and Technology, (242): 71-90. 2016. 10.1007/s00217-015-2520-0
- Serobatse, K. R. N.; Kabanda, M. M.
A theoretical study on the antioxidant properties of methoxy-substituted chalcone derivatives: A case study of kanakugiol and pedicellin through their Fe (II and III) coordination ability
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500486
- Setiawan, D.; Kalesky, R.; Kraka, E.; Cremer, D.
Direct Measure of Metal-Ligand Bonding Replacing the Tolman Electronic Parameter
Inorganic Chemistry, (55): 2332-2344. 2016. 10.1021/acs.inorgchem.5b02711
- Sexton, T.; Kraka, E.; Cremer, D.
Extraordinary Mechanism of the Diels-Alder Reaction: Investigation of Stereochemistry, Charge Transfer, Charge Polarization, and Biradicaloid Formation
Journal of Physical Chemistry A, (120): 1097-1111. 2016. 10.1021/acs.jpca.5b11493

Sexton, T. M.; Freindorf, M.; Kraka, E.; Cremer, D.
A Reaction Valley Investigation of the Cycloaddition of 1,3-Dipoles with the Dipolarophiles Ethene and Acetylene: Solution of a Mechanistic Puzzle
Journal of Physical Chemistry A, (120): 8400-8418. 2016. 10.1021/acs.jpca.6b07975

Seybold, P. G.
Computational estimation of the acidities of some inorganic nitrogen acids
Molecular Physics, (114): 389-393. 2016. 10.1080/00268976.2015.1076582

Seyedhosseini, B.; Izadyar, M.; Housaindokht, M. R.
DFT investigation on the selective complexation of ionic liquids based on alpha-amino acid anion and N7, N9-dimethyladeninium cation with CO₂
RSC Advances, (6): 85924-85932. 2016. 10.1039/c6ra15362c

Shabanian, M.; Moghanian, H.; Hajibeygi, M.; Mohamadi, A.
A DFT study of solvation effects and NBO analysis on the tautomerism of 1-substituted hydantoin
Arabian Journal of Chemistry, (9): S776-S780. 2016. 10.1016/j.arabjc.2011.08.014

Shah, M. I. A.; Xu, Z. Y.; Liu, L.; Jiang, Y. Y.; Shi, J.
Mechanism for the enhanced reactivity of 4-mercaptoprolyl thioesters in native chemical ligation
RSC Advances, (6): 68312-68321. 2016. 10.1039/c6ra13793h

Shah, P. K.; Bhattacharjee, K.; Shukla, P. K.
Mechanisms of reactions of Ru(III)-based drug NAMI-A and its aquated products with DNA purine bases: a DFT study
RSC Advances, (6): 113620-113629. 2016. 10.1039/c6ra24251k

Shah, S.; Hao, C.
Density functional theory study of direct and indirect photodegradation mechanisms of sulfamer
Environmental Science and Pollution Research, (23): 19921-19930. 2016. 10.1007/s11356-016-6956-y

Shahab, S.; Filippovich, L.; Borzehandani, M. Y.; Kumar, R.; Lugovsky, A.; Eryomin, A.; Mashayekhi, M.
IR-polarizing film containing a new quinoline dye and Fe₃O₄ nanoparticles: optical and thermophysical investigations
RSC Advances, (6): 114613-114622. 2016. 10.1039/c6ra23531j

Shahabi, M.; Raissi, H.
Investigation of the molecular structure, electronic properties, AIM, NBO, NMR and NQR parameters for the interaction of Sc, Ga and Mg-doped (6,0) aluminum nitride nanotubes with COCl₂ gas by DFT study
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (84): 99-114. 2016. 10.1007/s10847-015-0587-7

Shahabi, M.; Raissi, H.
Molecular dynamics simulation and quantum chemical studies on the investigation of aluminum nitride nanotube as phosgene gas sensor
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (86): 305-322. 2016. 10.1007/s10847-016-0664-6

Shahangi, F.; Chermahini, A. N.; Farrokhpour, H.; Dabbagh, H. A.
Enantiomeric discrimination of leucine enantiomers by nanotubular cyclic peptides: DFT and ONIOM calculation of the absorption spectra of guested enantiomers
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (85): 329-339. 2016. 10.1007/s10847-016-0632-1

Shaik, S.; Danovich, D.; Braida, B.; Hiberty, P. C.
The Quadruple Bonding in C-2 Reproduces the Properties of the Molecule
Chemistry-a European Journal, (22): 4116-4128. 2016. 10.1002/chem.201600011

Shaik, S.; Danovich, D.; Braida, B.; Wu, W.; Hiberty, P. C.
New Landscape of Electron-Pair Bonding: Covalent, Ionic, and Charge-Shift Bonds
Chemical Bond II: 100 Years Old and Getting Stronger, (170): 169-211. 2016. 10.1007/430_2015_179

- Shaikh, S. A. M.; Barik, A.; Singh, B. G.; Modukuri, R. V.; Balaji, N. V.; Subbaraju, G. V.; Naik, D. B.; Priyadarsini, K. I.
Free radical reactions of isoxazole and pyrazole derivatives of hispolon: kinetics correlated with molecular descriptors
Free Radical Research, (50): 1361-1373. 2016. 10.1080/10715762.2016.1247955
- Shainyan, B. A.; Chipanina, N. N.; Oznobikhina, L. P.; Meshcheryakov, V. I.
Basicity of trifluoromethylsulfonylformamidines. DFT and FTIR study and NBO analysis
Journal of Physical Organic Chemistry, (29): 92-100. 2016. 10.1002/poc.3503
- Shakerzadeh, E.; Khodayar, E.; Noorizadeh, S.
Theoretical assessment of phosgene adsorption behavior onto pristine, Al- and Ga-doped B12N12 and B16N16 nanoclusters
Computational Materials Science, (118): 155-171. 2016. 10.1016/j.commatsci.2016.03.016
- Shakourian-Fard, M.; Jamshidi, Z.; Kamath, G.
Surface Charge-Transfer Doping of Graphene Nanoflakes Containing Double-Vacancy (5-8-5) and Stone-Wales (55-77) Defects through Molecular Adsorption
Chemphyschem, (17): 3289-3299. 2016. 10.1002/cphc.201600614
- Shakourian-Fard, M.; Kamath, G.; Sankaranarayanan, S.
Evaluating the Free Energies of Solvation and Electronic Structures of Lithium-Ion Battery Electrolytes
Chemphyschem, (17): 2916-2930. 2016. 10.1002/cphc.201600338
- Shan, M. L.; Liu, Y. J.; Xia, S. W.; Tang, Q. W.; Yu, L. M.
A strategy of integrating ultraviolet absorption and crosslinking in a single molecule: DFT calculation and experimental
Journal of Molecular Structure, (1107): 249-253. 2016. 10.1016/j.molstruc.2015.11.049
- Shanmugam, R.; Thamaraiichelvan, A.; Ganesan, T. K.; Viswanathan, B.
Carbon dioxide activation and transformation to HCOOH on metal clusters ($M = Ni, Pd, Pt, Cu, Ag \& Au$) anchored on a polyaniline conducting polymer surface - an evaluation study by hybrid density functional theory
RSC Advances, (6): 100829-100840. 2016. 10.1039/c6ra20715d
- Sharafi-Kolkeshvandi, M.; Nematollahi, D.; Nikpour, F.; Bayat, M.; Soltani, E.
Electrochemical behavior of 2-aminodiphenylamine and efficient factors on the site-selectivity of sulfonylation reaction: Experimental and theoretical studies
Electrochimica Acta, (222): 845-855. 2016. 10.1016/j.electacta.2016.11.046
- Sharma, B.; Neela, Y. I.; Sastry, G. N.
Structures and Energetics of Complexation of Metal Ions with Ammonia, Water, and Benzene: A Computational Study
Journal of Computational Chemistry, (37): 992-1004. 2016. 10.1002/jcc.24288
- Sharma, C.; Singh, A. K.; Joy, J.; Jemmis, E. D.; Awasthi, S. K.
Experimental and theoretical study of intramolecular O center dot center dot center dot O interaction in structurally rigid beta-keto carboxylic esters
RSC Advances, (6): 91689-91693. 2016. 10.1039/c6ra20483j
- Sharon, D. A.; Mallick, D.; Wang, B. J.; Shaik, S.
Computation Sheds Insight into Iron Porphyrin Carbenes' Electronic Structure, Formation, and N-H Insertion Reactivity
Journal of the American Chemical Society, (138): 9597-9610. 2016. 10.1021/jacs.6b04636
- Shaw, R. A.; Hill, J. G.; Legon, A. C.
Halogen Bonding with Phosphine: Evidence for Mulliken Inner Complexes and the Importance of Relaxation Energy
Journal of Physical Chemistry A, (120): 8461-8468. 2016. 10.1021/acs.jpca.6b08945
- Shayan, K.; Nowroozi, A.
The first singlet excited state (S_1) intramolecular hydrogen bond of malonaldehyde derivatives: a TD-DFT and CIS study
Structural Chemistry, (27): 1769-1780. 2016. 10.1007/s11224-016-0796-8

Shchekotikhin, A. E.; Dezenkova, L. G.; Tsvetkov, V. B.; Luzikov, Y. N.; Volodina, Y. L.; Tatarskiy, V. V.; Kalinina, A. A.; Treshalin, M. I.; Treshalina, H. M.; Romanenko, V. I.; Kaluzhny, D. N.; Kubbutat, M.; Schols, D.; Pommier, Y.; Shtil, A. A.; Preobrazhenskaya, M. N.

Discovery of antitumor anthra 2,3-b furan-3-carboxamides: Optimization of synthesis and evaluation of antitumor properties

European Journal of Medicinal Chemistry, (112): 114-129. 2016. 10.1016/j.ejmech.2016.01.050

Sheikhi, A.; van de Ven, T. G. M.

Trapping It Softly: Ultrasoft Zirconium Metallogels for Macromolecule Entrapment and Reconfiguration

ACS Macro Letters, (5): 904-908. 2016. 10.1021/acsmacrolett.6b00447

Sheldon, J. E.; Dcona, M. M.; Lyons, C. E.; Hackett, J. C.; Hartman, M. C. T.

Photoswitchable anticancer activity via trans-cis isomerization of a combretastatin A-4 analog

Organic & Biomolecular Chemistry, (14): 40-49. 2016. 10.1039/c5ob02005k

Sheng, X. L.; Batista, E. R.; Duan, Y. X.; Tian, Y. H.

Dimension and bridging ligand effects on Mo-mediated catalytic transformation of dinitrogen to ammonia: Chain-like extended models of Nishibayashi's catalyst

Computational and Theoretical Chemistry, (1095): 134-141. 2016. 10.1016/j.comptc.2016.09.022

Sheong, F. K.; Chen, W. J.; Lin, Z. Y.

Lewis Description of Bonding in Transition Metal Complexes

Chemical Bond I: 100 Years Old and Getting Stronger, (169): 89-129. 2016. 10.1007/430_2015_182

Sheong, F. K.; Zhang, J. X.; Lin, Z. Y.

An Au-13 (5+) Approach to the Study of Gold Nanoclusters

Inorganic Chemistry, (55): 11348-11353. 2016. 10.1021/acs.inorgchem.6b01881

Sherin, D. R.; Manojkumar, T. K.; Rajasekharan, K. N.

CRANAD-1 as a cyanide sensor in aqueous media: a theoretical study

RSC Advances, (6): 99385-99390. 2016. 10.1039/c6ra19045f

Shewale, M. N.; Lande, D. N.; Gejji, S. P.

Encapsulation of benzimidazole derivatives within cucurbit 7 uril: Density functional investigations

Journal of Molecular Liquids, (216): 309-317. 2016. 10.1016/j.molliq.2015.12.076

Shi, G. Q.; Zhu, Y. C.; Wang, J.; Ren, Z. C.; Li, G.

Syntheses, structures and properties of four metal-organic frameworks from chlorophenyl imidazole dicarboxylates

Journal of Coordination Chemistry, (69): 2231-2246. 2016. 10.1080/00958972.2016.1197391

Shi, H. B.; Auerbach, S. M.; Ramasubramaniam, A.

First-Principles Predictions of Structure Function Relationships of Graphene-Supported Platinum Nanoclusters

Journal of Physical Chemistry C, (120): 11899-11909. 2016. 10.1021/acs.jpcc.6b01288

Shim, E. K. S.; Leong, W. K.; Li, Y. Z.; Richmond, M. G.

Isomerization of the osmium-tellurium cluster Os-3(mu-TeR)(2)(CO)(10): a kinetic and computational study

Dalton Transactions, (45): 7158-7162. 2016. 10.1039/c6dt00588h

Shiroudi, A.; Deleuze, M. S.

Reaction mechanisms and kinetics of the O-2 addition pathways to the main thiophene-OH adduct: a theoretical study

Progress in Reaction Kinetics and Mechanism, (41): 398-417. 2016. 10.3184/146867816x14754978258571

Shiroudi, A.; Zahedi, E.

Understanding the kinetics of thermal decomposition of 2,3-epoxy-2,3-dimethylbutane using RRKM theory

RSC Advances, (6): 91882-91892. 2016. 10.1039/c6ra21963b

Shohayeb, S. M.; Mohamed, R. G.; Moustafa, H.; El-Medani, S. M.

Synthesis, spectroscopic, DFT calculations and biological activity studies of ruthenium carbonyl complexes with 2-picolinic acid and a secondary ligand
Journal of Molecular Structure, (1119): 442-450. 2016. 10.1016/j.molstruc.2016.05.009

Shukla, A.; Khan, E.; Srivastava, A.; Tandon, P.; Sinha, K.
A computational study on molecular structure, multiple interactions, chemical reactivity and molecular docking studies on 6 D (-) -amino-phenyl-acetamido penicillanic acid(ampicillin)
Molecular Simulation, (42): 863-873. 2016. 10.1080/08927022.2015.1089996

Shukla, R.; Chopra, D.
Characterization of N center dot center dot O non-covalent interactions involving sigma-holes: "electrostatics" or "dispersion"
Physical Chemistry Chemical Physics, (18): 29946-29954. 2016. 10.1039/c6cp05899j

Shukla, R.; Chopra, D.
Crystallographic and Theoretical Investigation on the Nature and Characteristics of Type I C=S center dot center dot center dot S=C Interactions
Crystal Growth & Design, (16): 6734-6742. 2016. 10.1021/acs.cgd.6b01530

Shukla, R.; Chopra, D.
"Pnicogen bonds" or "chalcogen bonds": exploiting the effect of substitution on the formation of P center dot center dot center dot Se noncovalent bonds
Physical Chemistry Chemical Physics, (18): 13820-13829. 2016. 10.1039/c6cp01703g

Shukla, R.; Chopra, D.
Understanding the effect of substitution on the formation of S center dot center dot center dot F chalcogen bond
Journal of Chemical Sciences, (128): 1589-1596. 2016. 10.1007/s12039-016-1176-z

Shukla, V. K.; Al-Alshaikh, M. A.; El-Emam, A. A.; Sachan, A. K.; Srivastava, R.; Prasad, O.; Sinha, L.
Conformational search, spectral analysis and electronic properties of 5-(4-Pyridinyl)-1,3,4-thiadiazol-2-amine
Journal of Molecular Structure, (1108): 112-125. 2016. 10.1016/j.molstruc.2015.11.077

Shukla, V. K.; Sachan, A. K.; Pathak, S. K.; Srivastava, R.; Prasad, O.; Sinha, L.
Prediction of molecular properties and spectroscopic profile of Riluzole with different functionals (B3LYP, M06-2X, MPWLYP): A combined theoretical and experimental study
Journal of Molecular Structure, (1106): 265-276. 2016. 10.1016/j.molstruc.2015.10.088

Si, D. W.; Chen, K. X.; Yao, J.; Li, H. R.
Structures and Electronic Properties of Lithium Chelate-Based Ionic Liquids
Journal of Physical Chemistry B, (120): 3904-3913. 2016. 10.1021/acs.jpcb.6b00731

Si, H.; Zhang, C. Q.; Luo, X. L.; Chen, R.; Liang, G. M.
Theoretical studies on the hydrolysis mechanism of acetamiprid
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1830-z

Siadati, A.
A Theoretical Study on the Possibility of Functionalization of C-20 Fullerene Via its Diels-Alder Reaction with 1,3-Butadiene
Letters in Organic Chemistry, (13): 2-6. 2016. 10.2174/1570178612666151002002526

Siadati, S. A.
The Effect of Position Replacement of Functional Groups on the Stepwise character of 1,3-Dipolar Reaction of a Nitrile Oxide and an Alkene
Helvetica Chimica Acta, (99): 273-280. 2016. 10.1002/hlca.201500165

Siadati, S. A.
A Theoretical Study on Stepwise- and Concertedness of the Mechanism of 1,3-Dipolar Cycloaddition Reaction Between Tetra Amino Ethylene and Trifluoro Methyl Azide

Combinatorial Chemistry & High Throughput Screening, (19): 170-175. 2016. 10.2174/1386207319666151216145408

Siadati, S. A.; Amini-Fazl, M. S.; Babanezhad, E.

The possibility of sensing and inactivating the hazardous air pollutant species via adsorption and their 2+3 cycloaddition reactions with C-20 fullerene

Sensors and Actuators B-Chemical, (237): 591-596. 2016. 10.1016/j.snb.2016.06.125

Siadati, S. A.; Nami, N.

Investigation of the possibility of functionalization of C-20 fullerene by benzene via Diels-Alder reaction

Physica E-Low-Dimensional Systems & Nanostructures, (84): 55-59. 2016. 10.1016/j.physe.2016.05.041

Siadati, S. A.; Vessally, E.; Hosseini, A.; Edjlali, L.

Possibility of sensing, adsorbing, and destructing the Tabun-2D-skeletal (Tabun nerve agent) by C-20 fullerene and its boron and nitrogen doped derivatives

Synthetic Metals, (220): 606-611. 2016. 10.1016/j.synthmet.2016.08.003

Sibbald, P. A.

A theoretical analysis of substituent electronic effects on phosphine-borane bonds

Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3127-5

Siddiqui, K. A.; Lama, P.; Bienko, A.; Bienko, D.

Magneto-structural analysis of metal-ortoato coordination complexes based on N-H center dot center dot center dot O and O-H center dot center dot center dot O supramolecular synthon

Polyhedron, (111): 53-63. 2016. 10.1016/j.poly.2016.03.003

Sidhu, L. S.; Halder, A.; Rai, S.

Dopant induced modulation in the structure and electronic properties of Au-10 cluster

RSC Advances, (6): 87115-87123. 2016. 10.1039/c6ra20808h

Sidorenko, G. V.; Maltsev, D. A.; Miroslavov, A. E.; Suglobov, D. N.; Baranovskii, V. I.; Gurzhiy, V. V.; Lumpov, A. A.; Tyupina, M. Y.

Reactivity of higher technetium carbonyls in CO replacement: A quantum chemical analysis

Computational and Theoretical Chemistry, (1093): 55-66. 2016. 10.1016/j.comptc.2016.08.013

Sieranski, T.

The intricacies of the stacking interaction in a pyrrole-pyrrole system

Structural Chemistry, (27): 1107-1120. 2016. 10.1007/s11224-015-0732-3

Sifain, A. E.; Bjorgaard, J. A.; Myers, T. W.; Veauthier, J. M.; Chavez, D. E.; Prezhdo, O. V.; Scharff, R. J.; Tretiak, S.

Photoactive Excited States in Explosive Fe(II) Tetrazine Complexes: A Time-Dependent Density Functional Theory Study

Journal of Physical Chemistry C, (120): 28762-28773. 2016. 10.1021/acs.jpcc.6b10333

Silla, J. M.; Freitas, M. P.

Interactions affecting (1)J(C-F) SSCCs in neutral and ionic 2-, 3-and 4-fluoro-substituted piperidines: normal and reverse fluorine Perlin-like effect

RSC Advances, (6): 74598-74603. 2016. 10.1039/c6ra10272g

Silva, A. L. R.; Morais, V. M. F.; da Silva, M.; Simoes, R. G.; Bernardes, C. E. S.; Piedade, M. F. M.; da Piedade, M. E. M.

Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies

Journal of Chemical Thermodynamics, (95): 35-48. 2016. 10.1016/j.jct.2015.11.010

Silva, D. S.; Oliveira, B. G.

THE PARADIGM OF PROTON DONOR STRUCTURE ON HYDROGEN BOND FORMATION: C2H2 center dot center dot center dot 6(HF) COMPLEX

Quimica Nova, (39): 1085-1092. 2016. 10.21577/0100-4042.20160125

Silva, F. T.; Franco, C. H.; Favaro, D. C.; Freitas, L. H.; Moraes, C. B.; Ferreira, E. I.

Design, synthesis and antitrypanosomal activity of some nitrofurazone 1,2,4-triazolic bioisosteric analogues
European Journal of Medicinal Chemistry, (121): 553-560. 2016. 10.1016/j.ejmech.2016.04.065

Silva, J. D.; Angnes, R. A.; da Silva, V. H. M.; Servilha, B. M.; Adeel, M.; Braga, A. A. C.; Aponick, A.; Correia, C. R. D.
Intermolecular Noncovalent Hydroxy-Directed Enantioselective Heck Desymmetrization of Cyclopentenol:
Computationally Driven Synthesis of Highly Functionalized cis-4-Arylcyclopentenol Scaffolds
Journal of Organic Chemistry, (81): 2010-2018. 2016. 10.1021/acs.joc.5b02846

Silva, T. M.; Fiúza, S. M.; Marques, M. P. M.; de Carvalho, L.; Amado, A. M.
Conformational study and reassessment of the vibrational assignments for Norspermidine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (157): 227-237. 2016.
10.1016/j.saa.2016.01.003

Silva, W.; Silla, J. M.; Cormannich, R. A.; Fernandes, S. A.; Freitas, M. P.
The role of nonbonding interactions and the presence of fluoride on the conformational isomerism of 1,2-ethanediol
Chemical Physics, (473): 17-23. 2016. 10.1016/j.chemphys.2016.04.018

Silvi, B.
The Relevance of the ELF Topological Approach to the Lewis, Kossel, and Langmuir Bond Model
Chemical Bond II: 100 Years Old and Getting Stronger, (170): 213-247. 2016. 10.1007/430_2015_185

Silvi, B.; Ratajczak, H.
Hydrogen bonding and delocalization in the ELF analysis approach
Physical Chemistry Chemical Physics, (18): 27442-27449. 2016. 10.1039/c6cp05400e

Simler, T.; Frison, G.; Braunstein, P.; Danopoulos, A. A.
Direct synthesis of doubly deprotonated, dearomatised lutidine PNP Cr and Zr pincer complexes based on isolated K and Li ligand transfer reagents
Dalton Transactions, (45): 2800-2804. 2016. 10.1039/c6dt00144k

Singh, D. K.; Rathke, B.; Kiefer, J.; Materny, A.
Molecular Structure and Interactions in the Ionic Liquid 1-Ethyl-3-methylimidazolium Trifluoromethanesulfonate
Journal of Physical Chemistry A, (120): 6274-6286. 2016. 10.1021/acs.jpca.6b03849

Singh, R.; Sathe, V.; Sharma, A.; Kaur, S.; Saini, G. S. S.
Solvation of coumarin6 studied by vibrational spectroscopy and density functional theory
Journal of Molecular Structure, (1106): 170-180. 2016. 10.1016/j.molstruc.2015.10.073

Singh, R. N.; Rawat, P.; Sahu, S.; Kumar, Y.
Antimicrobial activity, structural evaluation and vibrational (FT-IR and FT-Raman) study of pyrrole containing vinyl derivatives
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (154): 47-57. 2016. 10.1016/j.saa.2015.09.032

Singh, S.; Singh, H.; Karthick, T.; Agarwal, P.; Erande, R. D.; Dethe, D. H.; Tandon, P.
Combine experimental and theoretical investigation on an alkaloid-Dimethylisoborreverine
Journal of Molecular Structure, (1103): 187-201. 2016. 10.1016/j.molstruc.2015.09.021

Singh, S. K.; Das, A.; Breton, G. W.
An ab Initio Study of the Effect of Substituents on the n -> pi Interactions between 7-Azaindole and 2,6-Difluorosubstituted Pyridines*
Journal of Physical Chemistry A, (120): 6258-6269. 2016. 10.1021/acs.jpca.6b03119

Singh, S. K.; Mishra, K. K.; Sharma, N.; Das, A.
Direct Spectroscopic Evidence for an n-pi Interaction*
Angewandte Chemie-International Edition, (55): 7801-7805. 2016. 10.1002/anie.201511925

Sirnidzija, P.; Lecours, M. J.; Marta, R. A.; Steinmetz, V.; McMahon, T. B.; Fillion, E.; Hopkins, W. S.
Changes in Tricarbastannatrane Transannular N-Sn Bonding upon Complexation Reveal Lewis Base Donicities

Inorganic Chemistry, (55): 9579-9585. 2016. 10.1021/acs.inorgchem.6b01185

Sivaramakrishna, A.; Sravani, C.; Venkatesh, S.; Pavankumar, B. B.; Vijayakrishna, K.; Bhat, H. R.; Jha, P. C.; Smith, G. S.
Theoretical and experimental investigations on stability and chemistry of organoiridium(III) complexes
RSC Advances, (6): 105528-105539. 2016. 10.1039/c5ra27350a

Sivarajani, T.; Periandy, S.; Xavier, S.
Conformational stability, molecular structure, vibrational, electronic, H-1 and C-13 spectral analysis of 3-pyridinemethanol using ab-initio/DFT method
Journal of Molecular Structure, (1108): 398-410. 2016. 10.1016/j.molstruc.2015.12.023

Siwatch, R. K.; Karwasara, S.; Sharma, M. K.; Mondal, S.; Mukherjee, G.; Rajaraman, G.; Nagendran, S.
Reactivity of LGe-NR2 and LGe(E)-NR2 over LGe-Cl and LGe(E)-Cl toward Me3SiX (L = Aminotroponiminate; NR2 = N(SiMe3)(2)/NC4H4; E = S/Se; X = Br/CN)
Organometallics, (35): 429-438. 2016. 10.1021/acs.organomet.5b00643

Skara, G.; Gimferrer, M.; De Proft, F.; Salvador, P.; Pinter, B.
Scrutinizing the Noninnocence of Quinone Ligands in Ruthenium Complexes: Insights from Structural, Electronic, Energy, and Effective Oxidation State Analyses
Inorganic Chemistry, (55): 2185-2199. 2016. 10.1021/acs.inorgchem.5b02543

Skoch, K.; Uhlik, F.; Cisarova, I.; Stepnicka, P.
Silver(I) complexes with 1'-(diphenylphosphino)-1-cyanoferrrocene: the art of improvisation in coordination
Dalton Transactions, (45): 10655-10671. 2016. 10.1039/c6dt01843b

Skourtis, S. S.; Liu, C. R.; Antoniou, P.; Virshup, A. M.; Beratan, D. N.
Dexter energy transfer pathways
Proceedings of the National Academy of Sciences of the United States of America, (113): 8115-8120. 2016.
10.1073/pnas.1517189113

Sliwa, P.; Kurleto, K.; Handzlik, J.; Rogalski, S.; Zak, P.; Wyrzykiewicz, B.; Pietraszuk, C.
Regioselectivity of Stoichiometric Metathesis of Vinylsilanes with Second-Generation Grubbs Catalyst: A Combined DFT and Experimental Study
Organometallics, (35): 621-628. 2016. 10.1021/acs.organomet.5b00878

Smiles, D. E.; Wu, G.; Hrobarik, P.; Hayton, T. W.
Use of Se-77 and Te-125 NMR Spectroscopy to Probe Covalency of the Actinide-Chalcogen Bonding in Th(E-n){N(SiMe3)(2)}(3) (-) (E = Se, Te; n=1, 2) and Their Oxo-Uranium(VI) Congeners
Journal of the American Chemical Society, (138): 814-825. 2016. 10.1021/jacs.5b07767

So, Y. M.; Li, Y.; Au-Yeung, K. C.; Wang, G. C.; Wong, K. L.; Sung, H. H. Y.; Arnold, P. L.; Williams, I. D.; Lin, Z. Y.; Leung, W. H.
Probing the Reactivity of the Ce=O Multiple Bond in a Cerium(IV) Oxo Complex
Inorganic Chemistry, (55): 10003-10012. 2016. 10.1021/acs.inorgchem.6b00480

Sobhi, C.; Nacereddine, A. K.; Nasri, L.; Lechtar, Z.; Djerourou, A.
A DFT study of the mechanism and the regioselectivity of 3+2 cycloaddition reactions of nitrile oxides with alpha,beta-acetylenic aldehyde
Molecular Physics, (114): 3193-3200. 2016. 10.1080/00268976.2016.1224395

Sohn, W. Y.; Brenner, V.; Gloaguen, E.; Mons, M.
Local NH-pi interactions involving aromatic residues of proteins: influence of backbone conformation and pi pi excitation on the pi H-bond strength, as revealed from studies of isolated model peptides*
Physical Chemistry Chemical Physics, (18): 29969-29978. 2016. 10.1039/c6cp04109d

Soleimannejad, J.; Nazarnia, E.
The effect of ligand substituent on crystal packing: Structural and theoretical studies of two Ga(III) supramolecular compounds
Journal of Molecular Structure, (1116): 207-217. 2016. 10.1016/j.molstruc.2016.03.047

- Soliman, I. M.; El-Nahass, M. M.; Eid, K. M.; Ammar, H. Y.
Vibrational spectroscopic analysis of aluminum phthalocyanine chloride. experimental and DFT study
Physica B-Condensed Matter, (491): 98-103. 2016. 10.1016/j.physb.2016.03.023
- Soliman, S. M.; Barakat, A.
Decomposition of Intermolecular Interactions in the Crystal Structure of Some Diacetyl Platinum(II) Complexes: Combined Hirshfeld, AIM, and NBO Analyses
Molecules, (21) 2016. 10.3390/molecules21121669
- Solimannejad, M.; Kamalinahad, S.; Shakerzadeh, E.
Selective detection of toxic cyanogen gas in the presence of O₂, and H₂O molecules using a AN nanocluster
Physics Letters A, (380): 2854-2860. 2016. 10.1016/j.physleta.2016.06.050
- Song, B. T.; Chu, Y. Y.; Li, G. C.; Wang, J. Q.; Lo, A. Y.; Zheng, A. M.; Deng, F.
Origin of Zeolite Confinement Revisited by Energy Decomposition Analysis
Journal of Physical Chemistry C, (120): 27349-27363. 2016. 10.1021/acs.jpcc.6b09059
- Song, X. W.; Fagiani, M. R.; Gewinner, S.; Schollkopf, W.; Asmis, K. R.; Bischoff, F. A.; Berger, F.; Sauer, J.
Gas phase structures and charge localization in small aluminum oxide anions: Infrared photodissociation spectroscopy and electronic structure calculations
Journal of Chemical Physics, (144) 2016. 10.1063/1.4954158
- Song, Z. J.
First-principle investigation on growth patterns and properties of cobalt-doped lithium nanoclusters
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3002-4
- Sorgenfrei, N.; Hioe, J.; Greindl, J.; Rothermel, K.; Morana, F.; Lokesh, N.; Gschwind, R. M.
NMR Spectroscopic Characterization of Charge Assisted Strong Hydrogen Bonds in Bronsted Acid Catalysis
Journal of the American Chemical Society, (138): 16345-16354. 2016. 10.1021/jacs.6b09243
- Soria-Martinez, R.; Mendoza-Merono, R.; Garcia-Granda, S.
Synthesis, crystal structure, spectroscopic characterization and theoretical study of (2E)-N-phenyl-2-(pyridin-3-ylmethylidene) hydrazinecarboxamide
Journal of Molecular Structure, (1105): 322-331. 2016. 10.1016/j.molstruc.2015.10.020
- Souza, M. L.; Roveda, A. C.; Pereira, J. C. M.; Franco, D. W.
New perspectives on the reactions of metal nitrosyls with thiolates as nucleophiles
Coordination Chemistry Reviews, (306): 615-627. 2016. 10.1016/j.ccr.2015.03.008
- Spallek, T.; Hess, O.; Meermann-Zimmermann, M.; Meermann, C.; Klimpel, M. G.; Estler, F.; Schneider, D.; Scherer, W.; Tafipolsky, M.; Tornroos, K. W.; Maichle-Mossmer, C.; Sirsch, P.; Anwander, R.
Synthesis and structural diversity of trivalent rare-earth metal diisopropylamide complexes
Dalton Transactions, (45): 13750-13765. 2016. 10.1039/c6dt01568a
- Spisak, S. N.; Li, J. B.; Rogachev, A. Y.; Wei, Z.; Papaianina, O.; Amsharov, K.; Rybalchenko, A. V.; Goryunkov, A. A.; Petrukhina, M. A.
From Corannulene to Indacenopicene: Effect of Carbon Framework Topology on Aromaticity and Reduction Limits
Organometallics, (35): 3105-3111. 2016. 10.1021/acs.organomet.6b00395
- Sponer, J. E.; Szabla, R.; Gora, R. W.; Saitta, A. M.; Pietrucci, F.; Saija, F.; Di Mauro, E.; Saladino, R.; Ferus, M.; Civis, S.; Sponer, J.
Prebiotic synthesis of nucleic acids and their building blocks at the atomic level - merging models and mechanisms from advanced computations and experiments
Physical Chemistry Chemical Physics, (18): 20047-20066. 2016. 10.1039/c6cp00670a
- Sprutta, N.; Welnic, M.; Bialek, M. J.; Lis, T.; Szterenberg, L.; Latos-Grazynski, L.
Carbocations Confined in a Thiatriazuliporphyrin Frame
Chemistry-a European Journal, (22): 6974-6980. 2016. 10.1002/chem.201504752

Srivastava, A.; Santhibhushan, B.; Sharma, V.; Kaur, K.; Khan, M. S.; Marathe, M.; De Sarkar, A.; Khan, M. S.
Influence of Boron Substitution on Conductance of Pyridine- and Pentane-Based Molecular Single Electron Transistors: First-Principles Analysis
Journal of Electronic Materials, (45): 2233-2241. 2016. 10.1007/s11664-015-4287-2

Srivastava, A. K.; Misra, N.
Can boron nitride analog of carbon nanoneedle exist?
Main Group Chemistry, (15): 191-196. 2016. 10.3233/mgc-150198

Srivastava, A. K.; Misra, N.
OLi₃O⁻ anion: Designing the strongest base to date using OLi₃ superalkali
Chemical Physics Letters, (648) 2016. 10.1016/j.cplett.2016.02.010

Srivastava, A. K.; Pandey, A. K.; Pandey, S.; Misra, N.
Structural, Electronic Properties, Hydrogen Bonding Analyses, and Biological Activity of Two Multiple Myeloma Drugs: Lenalidomide and Pomalidomide
Polycyclic Aromatic Compounds, (36): 452-466. 2016. 10.1080/10406638.2015.1011286

Srivastava, A. K.; Pandey, S. K.; Misra, N.
(CH₃Br center dot center dot center dot NH₃)@C-60: The effect of nanoconfinement on halogen bonding
Chemical Physics Letters, (662): 240-243. 2016. 10.1016/j.cplett.2016.09.036

Srivastava, A. K.; Pandey, S. K.; Misra, N.
Prediction of superalkali@C-60 endofullerenes, their enhanced stability and interesting properties
Chemical Physics Letters, (655): 71-75. 2016. 10.1016/j.cplett.2016.05.039

Srivastava, K.; Shimpi, M. R.; Srivastava, A.; Tandon, P.; Sinha, K.; Velaga, S. P.
Vibrational analysis and chemical activity of paracetamol-oxalic acid cocrystal based on monomer and dimer calculations: DFT and AIM approach
RSC Advances, (6): 10024-10037. 2016. 10.1039/c5ra24402a

Srivastava, K.; Srivastava, A.; Tandon, P.; Sinha, K.; Wang, J.
Spectroscopic, quantum chemical calculation and molecular docking of dipfluzine
Journal of Molecular Structure, (1125): 751-762. 2016. 10.1016/j.molstruc.2016.07.078

Srivastava, S.; Gupta, P.; Amandeep; Singh, R. P.
Synthesis of 4-((1E, 6E)-7-(4-hydroxy-3-methoxyphenyl)-3, 5-dioxohepta-1, 6-dienyl)-2-methoxyphenyl 4-fluorobenzoate, a novel monoester derivative of curcumin, its experimental and theoretical (DFT) studies
Journal of Molecular Structure, (1109): 58-66. 2016. 10.1016/j.molstruc.2015.12.029

Srivastava, S.; Gupta, P.; Sethi, A.; Singh, R. P.
One pot synthesis of Curcumin-NSAIDs prodrug, spectroscopic characterization, conformational analysis, chemical reactivity, intramolecular interactions and first order hyperpolarizability by DFT method
Journal of Molecular Structure, (1117): 173-180. 2016. 10.1016/j.molstruc.2016.03.033

Stachowicz-Kusnierz, A.; Korchowiec, J.
Nucleophilic properties of purine bases: inherent reactivity versus reaction conditions
Structural Chemistry, (27): 543-555. 2016. 10.1007/s11224-015-0583-y

Stasyuk, O. A.; Szatylowicz, H.; Krygowski, T. M.
Aromaticity of H-bonded and metal complexes of guanine tautomers
Structural Chemistry, (27): 111-118. 2016. 10.1007/s11224-015-0605-9

Stefanska, K.; Jedrzejewska, H.; Wierzbicki, M.; Szumna, A.; Iwanek, W.
The Inverse Demand Oxa-Diels-Alder Reaction of Resorcinarenes: An Experimental and Theoretical Analysis of Regioselectivity and Diastereoselectivity
Journal of Organic Chemistry, (81): 6018-6025. 2016. 10.1021/acs.joc.6b01099

- Stelzer, A. C.; Hrobarik, P.; Braun, T.; Kaupp, M.; Braun-Cula, B.
Completing the Heterocubane Family Cp^{}AlE (4) (E = O, S, Se, and Te) by Selective Oxygenation and Sulfuration of Cp^{*}Al (4): Density Functional Theory Calculations of Cp^{*}AlE (4) and Reactivity of (Cp^{*}AlO (4) toward Hydrolysis*
Inorganic Chemistry, (55): 4915-4923. 2016. 10.1021/acs.inorgchem.6b00462
- Stenlid, J. H.; Johansson, A. J.; Kloo, L.; Brinck, T.
Aqueous Solvation and Surface Oxidation of the Cu7 Nanoparticle: Insights from Theoretical Modeling
Journal of Physical Chemistry C, (120): 1977-1988. 2016. 10.1021/acs.jpcc.5b11361
- Stojanovic, M.; Baranac-Stojanovic, M.
Aromaticity of Diazaborines and Their Protonated Forms
Journal of Organic Chemistry, (81): 197-205. 2016. 10.1021/acs.joc.5b02499
- Su, J.; Li, W. L.; Lopez, G. V.; Jian, T.; Cao, G. J.; Li, W. L.; Schwarz, W. H. E.; Wang, L. S.; Li, J.
Probing the Electronic Structure and Chemical Bonding of Mono-Uranium Oxides with Different Oxidation States: UOx- and UOx (x=3-5)
Journal of Physical Chemistry A, (120): 1084-1096. 2016. 10.1021/acs.jpca.5b11354
- Su, P. F.; Chen, H. J.; Wu, W.
An energy decomposition analysis for intramolecular non-covalent interaction in solvated environment
Science China-Chemistry, (59): 1025-1032. 2016. 10.1007/s11426-016-0007-2
- Su, X.; Kulik, H. J.; Jamison, T. F.; Hatton, T. A.
Anion-Selective Redox Electrodes: Electrochemically Mediated Separation with Heterogeneous Organometallic Interfaces
Advanced Functional Materials, (26): 3394-3404. 2016. 10.1002/adfm.201600079
- Suardiaz, R.; Jambrina, P. G.; Masgrau, L.; Gonzalez-Lafont, A.; Rosta, E.; Lluch, J. M.
Understanding the Mechanism of the Hydrogen Abstraction from Arachidonic Acid Catalyzed by the Human Enzyme 15-Lipoxygenase-2. A Quantum Mechanics/Molecular Mechanics Free Energy Simulation
Journal of Chemical Theory and Computation, (12): 2079-2090. 2016. 10.1021/acs.jctc.5b01236
- Subashchandrabose, S.; Thanikachalam, V.; Manikandan, G.; Saleem, H.; Erdogan, Y.
Synthesis and spectral characterization of bis(4-amino-5-mercaptopro-1,2,4-triazol-3-yl)propane
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (157): 96-103. 2016.
10.1016/j.saa.2015.12.005
- Subashini, K.; Govindarajan, R.; Surendran, R.; Mukund, K.; Periandy, S.
Spectroscopic (FT-IR, FT-Raman, UV, NMR, NBO, NLO) investigation and molecular docking study of (R)-2-Methylamino-1-Phenylethanol (Halostachine)
Journal of Molecular Structure, (1125): 576-591. 2016. 10.1016/j.molstruc.2016.07.017
- Subashini, K.; Periandy, S.
Spectroscopic (FT-IR, FT-Raman, UV, NMR, NBO) investigation and molecular docking study of (R)-2-Amino-1-Phenylethanol
Journal of Molecular Structure, (1117): 240-256. 2016. 10.1016/j.molstruc.2016.03.063
- Sudharsana, N.; Sharma, A.; Kus, N.; Fausto, R.; Ramos, M. L.; Krishnakumar, V.; Pal, R.; Row, T. N. G.; Nagalakshmi, R.
Low temperature FTIR, Raman, NMR spectroscopic and theoretical study of hydroxyethylammonium picrate
Journal of Molecular Structure, (1104): 40-51. 2016. 10.1016/j.molstruc.2015.08.066
- Sugahara, T.; Guo, J. D.; Sasamori, T.; Karatsu, Y.; Furukawa, Y.; Ferao, A. E.; Nagase, S.; Tokitoh, N.
Reaction of a Stable Digermyne with Acetylenes: Synthesis of a 1,2-Digermabenzene and a 1,4-Digermabutrelene
Bulletin of the Chemical Society of Japan, (89): 1375-1384. 2016. 10.1246/bcsj.20160269
- Suganthi, S.; Balu, P.; Sathyaranayananamoorthi, V.; Kannappan, V.; Kamil, M. G. M.; Kumar, R.
Structural analysis and investigation of molecular properties of Cefpodoxime acid, a third generation antibiotic

Journal of Molecular Structure, (1108): 1-15. 2016. 10.1016/j.molstruc.2015.11.069

Suganthi, S.; Kannappan, V.; Sathyanarayananamoorthi, V.; Karunathan, R.

Quantum mechanical investigation of vibrational and electronic spectra of some 5-substituted isoquinolines

Indian Journal of Pure & Applied Physics, (54): 15-34. 2016.

Sukker, G. M.; Elroby, S. A.; Hilal, R.

Gas-phase acidity and dynamics of the protonation processes of carbidopa and levodopa. A QM/QD study
Journal of Biomolecular Structure & Dynamics, (34): 2268-2280. 2016. 10.1080/07391102.2015.1113385

Sukker, G. M.; Wazzan, N.; Ahmed, A.; Hilal, R.

Conformation and electronic structure of Carbidopa. A QM/MD study

Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500024

Sultan, M. A.; Karama, U.; Almansour, A. I.; Soliman, S. M.

Theoretical Study on Regioselectivity of the Diels-Alder Reaction between 1,8-Dichloroanthracene and Acrolein
Molecules, (21) 2016. 10.3390/molecules21101277

Sun, G.; Duan, X. X.; Liu, C. G.

The effect of Li doping on the nonlinear optical properties of 2,2 paracyclophane

Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-015-2879-7

Sun, H. C.; An, K.; Zhu, J.

Triplet State Aromaticity: NICS Criterion, Hyperconjugation, and Charge Effects

Chemistry-an Asian Journal, (11): 234-240. 2016. 10.1002/asia.201500897

Sun, H. T.; Cao, B. B.; Tian, Q. Q.; Liu, S. Y.; Du, D. M.; Xue, Z. M.; Fu, H.

A DFT study on the absorption mechanism of vinyl chloride by ionic liquids

Journal of Molecular Liquids, (215): 496-502. 2016. 10.1016/j.molliq.2016.01.026

Sun, J.; Dutta, T.; Parthasarathi, R.; Kim, K. H.; Tolic, N.; Chu, R. K.; Isern, N. G.; Cort, J. R.; Simmons, B. A.; Singh, S.

Rapid room temperature solubilization and depolymerization of polymeric lignin at high loadings

Green Chemistry, (18): 6012-6020. 2016. 10.1039/c6gc02258h

Sun, J.; Zheng, X. H.; He, H. T.; Chen, X.; Dong, B.; Fei, R.

Theoretical study of ligand and solvent effects on optical properties and stabilities of CdSe nanoclusters

Journal of Molecular Structure, (1114): 123-131. 2016. 10.1016/j.molstruc.2016.02.068

Sun, W. M.; Li, X. H.; Li, Y.; Liu, J. Y.; Wu, D.; Li, C. Y.; Ni, B. L.; Li, Z. R.

On the feasibility of designing hyperalkali cations using superalkali clusters as ligands

Journal of Chemical Physics, (145) 2016. 10.1063/1.4967461

Sun, W. M.; Li, X. H.; Li, Y.; Wu, D.; Li, C. Y.; Chen, J. H.; Li, Z. R.

Can Fluorinated Molecular Cages Be Utilized as Building Blocks of Hyperhalogens?

Chemphyschem, (17): 1468-1474. 2016. 10.1002/cphc.201600052

Sun, W. M.; Li, Y.; Li, X. H.; Wu, D.; He, H. M.; Li, C. Y.; Chen, J. H.; Li, Z. R.

Stability and Nonlinear Optical Response of Alkalides that Contain a Completely Encapsulated Superalkali Cluster

Chemphyschem, (17): 2672-2678. 2016. 10.1002/cphc.201600389

Sun, W. M.; Wu, D.; Li, X. H.; Li, Y.; Chen, J. H.; Li, C. Y.; Liu, J. Y.; Li, Z. R.

Quasi-Chalcogen Characteristics of Al₁₂Be: A New Member of the Three-Dimensional Periodic Table

Journal of Physical Chemistry C, (120): 2464-2471. 2016. 10.1021/acs.jpcc.5b11917

Sun, X.; Liu, X. J.; Xu, X. J.; Sun, P.

Molecular structure, spectroscopic, chemical reactivity, and nonlinear optical analysis of L-phenylalanine-benzoic acid optical crystals

Optik, (127): 4881-4888. 2016. 10.1016/j.ijleo.2016.02.015

- Sun, X. J.; Cao, B. B.; Zhou, X. M.; Liu, S. Y.; Zhu, X.; Fu, H.
Theoretical and experimental studies on proton transfer in acetate-based protic ionic liquids
Journal of Molecular Liquids, (221): 254-261. 2016. 10.1016/j.molliq.2016.05.080
- Sutradhar, D.; Chandra, A. K.; Zeegers-Huyskens, T.
Theoretical study of the interaction of fluorinated dimethyl ethers and the ClF and HF molecules. Comparison between halogen and hydrogen bonds
International Journal of Quantum Chemistry, (116): 670-680. 2016. 10.1002/qua.25083
- Suzuki, Y.; Sasamori, T.; Guo, J. D.; Nagase, S.; Tokitoh, N.
Isolation and Ambident Reactivity of a Chlorogermylenoid
Chemistry-a European Journal, (22): 13784-13788. 2016. 10.1002/chem.201602601
- Swenson, N. K.; Ratner, M. A.; Weiss, E. A.
Computational Study of the Resonance Enhancement of Raman Signals of Ligands Adsorbed to CdSe Clusters through Photoexcitation of the Cluster
Journal of Physical Chemistry C, (120): 20954-20960. 2016. 10.1021/acs.jpcc.6b02804
- Swiderski, G.; Lewandowska, H.; Swislocka, R.; Wojtulewski, S.; Siergiejczyk, L.; Wilczewska, A.
Thermal, spectroscopic (IR, Raman, NMR) and theoretical (DFT) studies of alkali metal complexes with pyrazinecarboxylate and 2,3-pyrazinedicarboxylate ligands
Journal of Thermal Analysis and Calorimetry, (126): 205-224. 2016. 10.1007/s10973-016-5695-0
- Szatkowski, L.; Hall, M. B.
Dehalogenation of chloroalkanes by nickel(I) porphyrin derivatives, a computational study
Dalton Transactions, (45): 16869-16877. 2016. 10.1039/c6dt02632j
- Szatylowicz, H.; Jeziorska, A.; Sadlej-Sosnowska, N.
Correlations of NBO energies of individual hydrogen bonds in nucleic acid base pairs with some QTAIM parameters
Structural Chemistry, (27): 367-376. 2016. 10.1007/s11224-015-0724-3
- Szatylowicz, H.; Siodla, T.; Stasyuk, O. A.; Krygowski, T. M.
Towards physical interpretation of substituent effects: the case of meta- and para-substituted anilines
Physical Chemistry Chemical Physics, (18): 11711-11721. 2016. 10.1039/c5cp06702b
- Szczepanik, D. W.
A new perspective on quantifying electron localization and delocalization in molecular systems
Computational and Theoretical Chemistry, (1080): 33-37. 2016. 10.1016/j.comptc.2016.02.003
- Szell, P. M. J.; Bryce, D. L.
Cl-35 Solid-State NMR and Computational Study of Chlorine Halogen Bond Donors in Single-Component Crystalline Chloronitriles
Journal of Physical Chemistry C, (120): 11121-11130. 2016. 10.1021/acs.jpcc.6b02806
- Tahan, A.; Khojandi, M.; Salari, A. A.
The theoretical investigation of solvent effects on the relative stability and N-15 NMR shielding of antidepressant heterocyclic drug
Russian Journal of Physical Chemistry A, (90): 130-135. 2016. 10.1134/s0036024416010039
- Taherpour, A.; Rahimizadeh, R.
Study of solvent effects on structural and conformational properties of cimetidine tautomers
Medicinal Chemistry Research, (25): 2042-2057. 2016. 10.1007/s00044-016-1612-0
- Taimoori, S. M.; Dudding, T.
An Evolving Insight into Chiral H-Bond Catalyzed Aza-Henry Reactions: A Cooperative Role for Noncovalent Attractive Interactions Unveiled by Density Functional Theory
Journal of Organic Chemistry, (81): 3286-3295. 2016. 10.1021/acs.joc.6b00248

- Tajabadi, J.; Bakavoli, M.; Gholizadeh, M.; Eshghi, H.
A mechanistic insight into the effect of piperidine as an organocatalyst on the 3+2 cycloaddition reaction of benzalacetone with phenyl azide from a computational study
Organic & Biomolecular Chemistry, (14): 7324-7333. 2016. 10.1039/c6ob00815a
- Talipov, M. R.; Hossain, M. M.; Boddeda, A.; Thakur, K.; Rathore, R.
A search for blues brothers: X-ray crystallographic/spectroscopic characterization of the tetraaryl-benzidine cation radical as a product of aging of solid magic blue
Organic & Biomolecular Chemistry, (14): 2961-2968. 2016. 10.1039/c6ob00140h
- Tamer, O.; Arslan, B. S.; Avci, D.; Nebioglu, M.; Atalay, Y.; Cosut, B.
Synthesis, molecular structure, spectral analysis and nonlinear optical studies on 4-(4-bromophenyl)-1-tert-butyl-3-methyl-1H-pyrazol-5-amine: A combined experimental and DFT approach
Journal of Molecular Structure, (1106): 89-97. 2016. 10.1016/j.molstruc.2015.10.084
- Tamer, O.; Atalay, A. S.; Avci, D.; Atalay, Y.; Tarcan, E.; Marchewka, M. K.
Optimized geometry, vibration (IR and Raman) spectra and nonlinear optical activity of p-nitroanilinium perchlorate molecule: A theoretical study
Materials Science-Poland, (34): 192-203. 2016. 10.1515/msp-2016-0002
- Tamer, O.; Avci, D.; Atalay, Y.
Synthesis, X-Ray crystal structure, photophysical characterization and nonlinear optical properties of the unique manganese complex with picolinate and 1,10 phenanthroline: toward the designing of new high NLO response crystal
Journal of Physics and Chemistry of Solids, (99): 124-133. 2016. 10.1016/j.jpcs.2016.08.013
- Tamer, O.; Avci, D.; Atalay, Y.; Cosut, B.; Zorlu, Y.; Erkovan, M.; Yerli, Y.
Synthesis, crystal structure, spectroscopic characterization and nonlinear optical properties of manganese (II) complex of picolinate: A combined experimental and computational study
Journal of Molecular Structure, (1106): 98-107. 2016. 10.1016/j.molstruc.2015.10.077
- Tamer, O.; Bhatti, M. H.; Yunus, U.; Avci, D.; Atalay, Y.; Nadeem, M.; Shah, S. R.; Hellwell, M.
Structural, spectroscopic, nonlinear optical and electronic properties of calcium N-phthaloylglycinate: A combined experimental and theoretical study
Journal of Molecular Structure, (1125): 315-322. 2016. 10.1016/j.molstruc.2016.06.084
- Tan, J. J.; Gong, S. D.; Deng, J. M.; Li, Q. S.; Luo, Q.; Xie, Y. M.; King, R. B.
Energetic preference of dative fluorine-manganese bonds over direct manganese-manganese bonds in binuclear hexafluorocyclopentadiene manganese carbonyls
Journal of Fluorine Chemistry, (188): 50-57. 2016. 10.1016/j.jfluchem.2016.06.003
- Tanak, H.; Kocak, F.; Agar, E.
A combined experimental (XRD, FT-IR, and UV-Vis) and DFT computational studies on (E)-N- 4-bromo-2-(trifluoromethoxy) phenyl -1-(5-nitrothiophen-2-yl) methanimine
Molecular Physics, (114): 197-212. 2016. 10.1080/00268976.2015.1090636
- Tanak, H.; Pawlus, K.; Marchewka, M. K.
Molecular structure, vibrational spectra and DFT computational studies of melaminium N-acetylglycinate dihydrate
Journal of Molecular Structure, (1121): 142-155. 2016. 10.1016/j.molstruc.2016.05.059
- Tanaka, H.; Nishibayashi, Y.; Yoshizawa, K.
Interplay between Theory and Experiment for Ammonia Synthesis Catalyzed by Transition Metal Complexes
Accounts of Chemical Research, (49): 987-995. 2016. 10.1021/acs.accounts.6b00033
- Tanase, T.; Koike, K.; Uegaki, M.; Hatada, S.; Nakamae, K.; Kure, B.; Ura, Y.; Nakajima, T.
Electron-rich linear triplatinum complexes stabilized by a spinning tetraphosphine, tris(diphenylphosphinomethyl)phosphine
Dalton Transactions, (45): 7209-7214. 2016. 10.1039/c6dt00624h

- Tang, C. M.; Wang, Z. G.; Zhang, X.; Wen, N. H.
The hydrogen storage properties of Na decorated small boron cluster B6Na8
Chemical Physics Letters, (661): 161-167. 2016. 10.1016/j.cplett.2016.08.064
- Tang, F.; Jia, J. F.; Wu, H. S.
The interaction of H-2 with multidecker C6-nBnH6Sc (n=0-6) complexes
Computational Materials Science, (112): 327-332. 2016. 10.1016/j.commatsci.2015.11.005
- Tang, M.; Zeng, Z. Y.; Cheng, Y.; Chen, X. R.; Cai, L. C.
Ab initio investigation of structure, stability, polarizability, and electronic structure of Ga4As4 cluster
Computational and Theoretical Chemistry, (1084): 109-118. 2016. 10.1016/j.comptc.2016.03.027
- Tang, Q. J.; Li, Q. Z.
Enhancing effect of metal coordination interaction on pnicogen bonding
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2929-9
- Tang, S. S.; Zhao, H. L.; Du, L.
Hydrogen bonding in alcohol-ethylene oxide and alcohol-ethylene sulfide complexes
RSC Advances, (6): 91233-91242. 2016. 10.1039/c6ra16205c
- Tanoury, G. J.
Chemoselective intermolecular hydrogen bonding in peptides: An electronic and topological study on the H-bonding selectivities in peptidomimetic HCV protease inhibitor telaprevir
Computational and Theoretical Chemistry, (1084): 140-149. 2016. 10.1016/j.comptc.2016.03.022
- Tantardini, C.; Boldyreva, E. V.; Benassi, E.
Hypervalency in Organic Crystals: A Case Study of the Oxicam Sulfonamide Group
Journal of Physical Chemistry A, (120): 10289-10296. 2016. 10.1021/acs.jpca.6b10703
- Tao, Y.; Xu, L. J.; Zhang, Z.; Chen, R. F.; Li, H. H.; Xu, H.; Zheng, C.; Huang, W.
Achieving Optimal Self-Adaptivity for Dynamic Tuning of Organic Semiconductors through Resonance Engineering
Journal of the American Chemical Society, (138): 9655-9662. 2016. 10.1021/Jacs.6b05042
- Tarakanov, P. A.; Simakov, A. O.; Dzuban, A. V.; Shestov, V. I.; Tarakanova, E. N.; Pushkarev, V. E.; Tomilova, L. G.
5,7-Bis(2'-arylethenyl)-6H-1,4-diazepine-2,3-dicarbonitriles: synthesis, and experimental and theoretical evaluation of the effects of substituents at 5,6,7-positions on the molecular configuration and spectral properties
Organic & Biomolecular Chemistry, (14): 1138-1146. 2016. 10.1039/c5ob02098k
- Tarakanova, E. N.; Trashin, S. A.; Simakov, A. O.; Furuyama, T.; Dzuban, A. V.; Inasaridze, L. N.; Tarakanov, P. A.; Troshin, P. A.; Pushkarev, V. E.; Kobayashi, N.; Tomilova, L. G.
Double-decker bis(tetradiazepinoporphyrazinato) rare earth complexes: crucial role of intramolecular hydrogen bonding
Dalton Transactions, (45): 12041-12052. 2016. 10.1039/c6dt01779g
- Tavakkoli, H.; Farhadipour, A.
Mononuclear gallium (III) complexes based on salicylaldoximes: Theoretical study of structures, topological and NBO analysis of hydrogen bonding interactions involving O-H center dot center dot center dot O bonds
Arabian Journal of Chemistry, (9): S361-S372. 2016. 10.1016/j.arabjc.2011.05.001
- Tavhare, P.; Wadnerkar, N.; Kalamse, V.; Chaudhari, A.
H-2 Interaction with C2H2TM (TM = Sc, Ti, V) Complex Using Quantum Chemical Methods
Acta Physica Polonica A, (129): 1257-1262. 2016. 10.12693/APhysPolA.129.1257
- Tay, M. Q. Y.; Ilic, G.; Werner-Zwanziger, U.; Lu, Y. P.; Ganguly, R.; Ricard, L.; Frison, G.; Carmichael, D.; Vidovic, D.
Preparation, Structural Analysis, and Reactivity Studies of Phosphenium Dications
Organometallics, (35): 439-449. 2016. 10.1021/acs.organomet.5b00763

- Tchougreeff, A. L.; Dronskowski, R.
Two theorems about C-2 and some more
Molecular Physics, (114): 1423-1444. 2016. 10.1080/00268976.2016.1158422
- Tellez, C. A.; Costa, A. C.; Mondragon, M. A.; Ferreira, G. B.; Versiane, O.; Rangel, J. L.; Lima, G. M.; Martin, A. A.
Molecular structure, natural bond analysis, vibrational and electronic spectra, surface enhanced Raman scattering and Mulliken atomic charges of the normal modes of Mn(DDTC)(2) complex
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (169): 95-107. 2016.
10.1016/j.saa.2016.06.018
- Terranova, Z. L.; Paesani, F.
The effects of framework dynamics on the behavior of water adsorbed in the Zn(I-L)(Cl) and Co-MOF-74 metal-organic frameworks
Physical Chemistry Chemical Physics, (18): 8196-8204. 2016. 10.1039/c5cp07681a
- Teyar, B.; Belkhiri, L.; Costuas, K.; Boucekkine, A.; Meyer, K.
Electronic Structure and Magnetic Properties of Dioxo-Bridged Diuranium Complexes with Diamond-Core Structural Motifs: A Relativistic DFT Study
Inorganic Chemistry, (55): 2870-2881. 2016. 10.1021/acs.inorgchem.5b02704
- Thangavel, S.; Boopathi, S.; Mahadevaiah, N.; Kolandaiyel, P.; Pansuriya, P. B.; Friedrich, H. B.
Catalytic oxidation of primary aromatic alcohols using half sandwich Ir(III), Rh(III) and Ru(II) complexes: A practical and theoretical study
Journal of Molecular Catalysis a-Chemical, (423): 160-171. 2016. 10.1016/j.molcata.2016.06.017
- Thatcher, R. J.; Johnson, D. G.; Slattery, J. M.; Douthwaite, R. E.
Structure of Amido Pyridinium Betaines: Persistent Intermolecular C-HN Hydrogen Bonding in Solution
Chemistry-a European Journal, (22): 3414-3421. 2016. 10.1002/chem.201503884
- Thirunarayanan, S.; Arjunan, V.; Marchewka, M. K.; Mohan, S.; Atalay, Y.
Characterisation of 1,3-diammonium propylselenate monohydrate by XRD, FT-IR, FT-Raman, DSC and DFT studies
Journal of Molecular Structure, (1107): 220-230. 2016. 10.1016/j.molstruc.2015.11.052
- Thompson, M. C.; Weber, J. M.
Infrared spectroscopic studies on the cluster size dependence of charge carrier structure in nitrous oxide cluster anions
Journal of Chemical Physics, (144) 2016. 10.1063/1.4943189
- Thong, N. M.; Ngo, T. C.; Dao, D. Q.; Duong, T.; Tran, Q. T.; Nam, P. C.
Functionalization of fullerene via the Bingel reaction with alpha-chlorocarbonanions: an ONIOM approach
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2981-5
- Tiago, F. S.; Santiago, P. H. O.; Amaral, M. M. P.; Martins, J. B. L.; Gatto, C. C.
New Cu(II) complex with acetylpyridine benzoyl hydrazone: experimental and theoretical analysis
Journal of Coordination Chemistry, (69): 330-342. 2016. 10.1080/00958972.2015.1105367
- Tian, W. J.; Chen, Q.; Li, H. R.; Yan, M.; Mu, Y. W.; Lu, H. G.; Zhai, H. J.; Li, S. D.
Saturn-like charge-transfer complexes Li-4&B-36, Li-5&B-36(+), and Li-6&B-36(2+): exohedral metallocaborospherenes with a perfect cage-like B-36(4-) core
Physical Chemistry Chemical Physics, (18): 9922-9926. 2016. 10.1039/c6cp01279e
- Tian, Y.; Fu, J.; Zhang, Y.; Li, B.; Bai, C. Y.; Cao, K. C.; Zhang, S.; Zhao, X. S.; Li, Y.; Wang, L.; Luo, Y.; Wang, D. Q.; Li, S. J.; Ma, L. J.; Xue, Y.
Insight Into the Influence of Ligand Conformation on Extraction Behaviour of Uranium: A Combined Theoretical and Experimental Study
Journal of Nanoscience and Nanotechnology, (16): 9603-9611. 2016. 10.1166/jnn.2016.12036
- Tikhonov, S. A.; Vovna, V. I.; Borisenko, A. V.
Photoelectron spectra and electronic structure of nitrogen analogues of boron beta-diketonates

Journal of Molecular Structure, (1115): 1-7. 2016. 10.1016/j.molstruc.2016.02.075

Toda, T.; Yoshinari, A.; Ikariya, T.; Kuwata, S.

Protic N-Heterocyclic Carbene Versus Pyrazole: Rigorous Comparison of Proton- and Electron-Donating Abilities in a Pincer-Type Framework

Chemistry-a European Journal, (22): 16675-16683. 2016. 10.1002/chem.201602552

Tofan, D.; Gabbai, F. P.

Fluorinated antimony(V) derivatives: strong Lewis acidic properties and application to the complexation of formaldehyde in aqueous solutions

Chemical Science, (7): 6768-6778. 2016. 10.1039/c6sc02558g

Tognetti, V.; Joubert, L.

Unraveling charge transfer processes with the quantum theory of atoms-in-molecules

Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1873-1

Tognetti, V.; Loos, P. F.

Natural occupation numbers in two-electron quantum rings

Journal of Chemical Physics, (144) 2016. 10.1063/1.4940919

Tolan, R. V.; Lupan, A.; Silaghi-Dumitrescu, R.

Computational Study on the Effect of Axial Ligation Upon the Electronic Structure of Copper (II) Porphyrinate (CuTPPs = 5,10,15,20-tetrakis(N-methylpyridyl-4)porphinato copper(II)tetratosylate)) - Electronic Structure with Different Axial Ligands

Journal of the Chemical Society of Pakistan, (38): 405-414. 2016.

Toldo, J. M.; Merlo, A. A.; Goncalves, P. F. B.

The 1,3-Dipolar Cycloaddition of Nitrile Oxide to Vinylacetic Acid: Computational Study of Transition States Selectivity, Solvent Effects, and Bicyclo Formation

Journal of the Brazilian Chemical Society, (27): 1202-1216. 2016. 10.5935/0103-5053.20160016

Toma, A.; Rat, C. I.; Silvestru, A.; Ruffer, T.; Lang, H.; Mehring, M.

Heterocyclic bismuth(III) compounds with transannular S → Bi interactions. An experimental and theoretical approach

Journal of Organometallic Chemistry, (806): 5-11. 2016. 10.1016/j.jorgchem.2016.01.019

Toma, Y.; Kunigami, M.; Watanabe, K. J.; Higashi, M.; Arimitsu, S.

One-pot synthesis and theoretical calculation for trifluoromethylated pyrrolizidines by 1,3-dipolar cycloaddition with azomethine ylides and beta-trifluoromethyl acrylamides

Journal of Fluorine Chemistry, (189): 22-32. 2016. 10.1016/j.jfluchem.2016.07.013

Toosy, N. K. A.; Raissi, H.; Zaboli, M.

Theoretical calculations of intramolecular hydrogen bond of the 2-Amino-2, 4, 6-cycloheptatrien-1-one in the gas phase and solution: Substituent effects and their positions

Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500632

Tormena, C. F.

Conformational analysis of small molecules: NMR and quantum mechanics calculations

Progress in Nuclear Magnetic Resonance Spectroscopy, (96): 73-88. 2016. 10.1016/j.pnmrs.2016.04.001

Transue, W. J.; Velian, A.; Nava, M.; Martin-Drumel, M. A.; Womack, C. C.; Jiang, J.; Hou, G. L.; Wang, X. B.; McCarthy, M. C.; Field, R. W.; Cummins, C. C.

A Molecular Precursor to Phosphaethyne and Its Application in Synthesis of the Aromatic 1,2,3,4-Phosphatriazolate Anion

Journal of the American Chemical Society, (138): 6731-6734. 2016. 10.1021/jacs.6b03910

Trofimov, B. A.; Andriyankova, L. V.; Nikitina, L. P.; Belyaeva, K. V.; Mal'kina, A. G.; Afonin, A. V.; Ushakov, I. A.; Kobychev, V. B.; Muzalevskiy, V. M.; Nenajdenko, V. G.

Reaction of imidazole derivatives with trifluoromethylated arylacetylenes

Journal of Fluorine Chemistry, (188): 157-163. 2016. 10.1016/j.jfluchem.2016.06.013

Troian-Gautier, L.; Beauvilliers, E. E.; Swords, W. B.; Meyer, G. J.

Redox Active Ion-Paired Excited States Undergo Dynamic Electron Transfer

Journal of the American Chemical Society, (138): 16815-16826. 2016. 10.1021/jacs.6b11337

Trujillo, C.; Previtali, V.; Rozas, I.

A theoretical model of the interaction between phosphates in the ATP molecule and guanidinium systems

Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-2012-8

Trujillo, C.; Sanchez-Sanz, G.

A Study of pi-pi Stacking Interactions and Aromaticity in Polycyclic Aromatic Hydrocarbon/Nucleobase Complexes

Chemphyschem, (17): 395-405. 2016. 10.1002/cphc.201501019

Tsuji, Y.; Hoffmann, R.; Miller, J. S.

Revisiting Ir(CO)(3)Cl

Polyhedron, (103): 141-149. 2016. 10.1016/j.poly.2015.09.050

Tsukada, S.; O'Brien, N. J.; Kano, N.; Kawashima, T.; Guo, J. D.; Nagase, S.

The synthesis and structure of a dianionic species with a bond between pentacoordinated tin atoms: bonding properties of the tin-tin bond

Dalton Transactions, (45): 19374-19379. 2016. 10.1039/c6dt03503e

Tyunina, V. V.; Krasnov, A. V.; Badelin, V. G.; Girichev, G. V.

Enthalpy of sublimation of hydroxyl-containing amino acids: Knudsen's effusion mass spectrometric study

Journal of Chemical Thermodynamics, (98): 62-70. 2016. 10.1016/j.jct.2016.02.021

Uddin, K. M.; Henry, D. J.

Further Theoretical Studies of the Aquation of Chromium(III) Chloride Nutritional Supplement: Effect of pH and Solvation

Chemistryselect, (1): 5236-5249. 2016. 10.1002/slct.201601305

Uddin, K. M.; Poirier, R. A.; Henry, D. J.

Mechanistic study of the aquation of nutritional supplement chromium chloride and other chromium(III) dihalides

Computational and Theoretical Chemistry, (1084): 88-97. 2016. 10.1016/j.comptc.2016.03.016

Uddin, M. M.; Begum, N.; Ghosh, S.; Sarker, J. C.; Tocher, D. A.; Hogarth, G.; Richmond, M. G.; Nordlander, E.; Kabir, S. E.

Thermal transformations of tris(2-thienyl)phosphine (PTh3) at low-valent ruthenium cluster centers: Part I. Carbon hydrogen, carbon phosphorus and carbon sulfur bond activation yielding Ru-3(CO)(8)L{mu-Th2P(C4H2S)}{mu-H} (L = CO, PTh3), Ru-3(CO)(7){mu-PTh2}(2){mu(3)-eta(2)-C4H2S}, Ru-4(CO)(9){mu-CO}(2){mu 4-eta(2)-C4H2S}{mu(4)-PTh} and Ru-5(CO)(11){mu-PTh2}{mu(4)-eta(4)-C4H3}{mu(4)-S}

Journal of Organometallic Chemistry, (812): 197-206. 2016. 10.1016/j.jorganchem.2015.06.026

Ugarte, R. A.; Devarajan, D.; Mushinski, R. M.; Hudnall, T. W.

Antimony(v) cations for the selective catalytic transformation of aldehydes into symmetric ethers, alpha, beta-unsaturated aldehydes, and 1,3,5-trioxanes

Dalton Transactions, (45): 11150-11161. 2016. 10.1039/c6dt02121b

Ulloa, O. A.; Huynh, M. T.; Richers, C. P.; Bertke, J. A.; Nilges, M. J.; Hammes-Schiffer, S.; Rauchfuss, T. B.

Mechanism of H-2 Production by Models for the NiFe -Hydrogenases: Role of Reduced Hydrides

Journal of the American Chemical Society, (138): 9234-9245. 2016. 10.1021/jacs.6b04579

Unluer, D.; Unver, Y.; Dugdu, E.; Akcay, H. T.; Sancak, K.

4-(4-((5-Amino-1,3,4-thiadiazol-2-yl)methoxy) phenyl)-1-((5-amino-1,3,4-thiadiazol-2-yl)methyl)-3-benzyl-1H-1,2,4-triazol-5(H)-one: Synthesis, Characterization and Computational Studies

Letters in Organic Chemistry, (13): 604-617. 2016. 10.2174/1570178613666160930121719

Ustynyuk, Y. A.; Alyapyshev, M. Y.; Babain, V. A.; Ustynyuk, N. A.

Quantum chemical modelling of extraction separation of minor actinides and lanthanides: the state of the art
Russian Chemical Reviews, (85): 917-942. 2016. 10.1070/rccr4588

Usui, K.; Irle, S.; Yokogawa, D.

Understanding of the Off-On Response Mechanism in Caged Fluorophores Based on Quantum and Statistical Mechanics
Journal of Physical Chemistry B, (120): 4449-4456. 2016. 10.1021/acs.jpcb.6b02298

Uzunova, E. L.; Mikosch, H.

Adsorption of phosphates and phosphoric acid in zeolite clinoptilolite: Electronic structure study
Microporous and Mesoporous Materials, (232): 119-125. 2016. 10.1016/j.micromeso.2016.06.019

Uzunova, E. L.; Mikosch, H.

A theoretical study of nitric oxide adsorption and dissociation on copper-exchanged zeolites SSZ-13 and SAPO-34: the impact of framework acid-base properties
Physical Chemistry Chemical Physics, (18): 11233-11242. 2016. 10.1039/c6cp01146b

Vach, H.; Ivanova, L. V.; Timerghazin, Q. K.; Jardali, F.; Le, H. L. T.

Metallic-like bonding in plasma-born silicon nanocrystals for nanoscale bandgap engineering
Nanoscale, (8): 18062-18069. 2016. 10.1039/c6nr04349f

Valdez, C. E.; Morgenstern, A.; Eberhart, M. E.; Alexandrova, A. N.

Predictive methods for computational metalloenzyme redesign - a test case with carboxypeptidase A
Physical Chemistry Chemical Physics, (18): 31744-31756. 2016. 10.1039/c6cp02247b

Valiev, M.; Deng, S. H. M.; Wang, X. B.

How Anion Chaotrope Changes the Local Structure of Water: Insights from Photoelectron Spectroscopy and Theoretical Modeling of SCN- Water Clusters
Journal of Physical Chemistry B, (120): 1518-1525. 2016. 10.1021/acs.jpcb.5b07257

van Rensburg, A. J.; Landman, M.; van Rooyen, P. H.; Marrigje, M.; Conradie, J.

Synthesis and structure of novel triphenylarsine-substituted tungsten(0) Fischer carbene complexes
Journal of Molecular Structure, (1105): 205-213. 2016. 10.1016/j.molstruc.2015.10.012

Vanzin, D.; Freitas, C. F.; Pellosi, D. S.; Batistela, V. R.; Machado, A. E. H.; Pontes, R. M.; Caetano, W.; Hioka, N.

Experimental and computational studies of protolytic and tautomeric equilibria of Erythrosin B and Eosin Y in water/DMSO
RSC Advances, (6): 110312-110328. 2016. 10.1039/c6ra12198e

Vasquez-Espinal, A.; Pino-Rios, R.; Fuentealba, P.; Orellana, W.; Tiznado, W.

Insights into the hydrogen dissociation mechanism on lithium edge-decorated carbon rings and graphene nanoribbon
International Journal of Hydrogen Energy, (41): 5709-5715. 2016. 10.1016/j.ijhydene.2016.02.018

Vatanparast, M.; Parvini, E.; Bahadori, A.

Computational study of the cooperative effects between tetrel bond and halogen bond in XCN center dot center dot center dot F2CO center dot center dot center dot YCN complexes (X = H, F, Cl, Br; Y = F, Cl, Br)
Molecular Physics, (114): 1478-1484. 2016. 10.1080/00268976.2015.1136005

Vektariene, A.

Theoretical study on the mechanism of thieno 3,2-b benzofuran bromination: the importance of Lewis and non-Lewis type NBOs interactions along the reaction path
Journal of Physical Organic Chemistry, (29): 21-28. 2016. 10.1002/poc.3483

Velazquez, J. D. H.; Barroso-Flores, J.; Goicochea, A. G.

Ab Initio Modeling Of Friction Reducing Agents Shows Quantum Mechanical Interactions Can Have Macroscopic Manifestation
Journal of Physical Chemistry A, (120): 9244-9248. 2016. 10.1021/acs.jpca.6b07890

Velez, E.; Ruiz, P.; Quijano, J.; Notario, R.

Gas-Phase Elimination Reaction of Ethyl (5-cyanomethyl-1,3,4-thiadiazol-2-yl) carbamate: A Computational Study
International Journal of Chemical Kinetics, (48): 23-31. 2016. 10.1002/kin.20967

Venkatesh, G.; Govindaraju, M.; Vennila, P.

Experimental and theoretical spectral investigations of 5-chloro-ortho-methoxyaniline using FT-IR, FT-Raman and DFT analysis

Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (55): 413-422. 2016.

Venkatesh, G.; Govindaraju, M.; Vennila, P.; Kamal, C.

Molecular structure, vibrational spectral assignments (FT-IR and FT-RAMAN), NMR, NBO, HOMO-LUMO and NLO properties of 2-nitroacetophenone based on DFT calculations
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500073

Venkatesh, S.; Sravani, C.; Janardan, S.; Suman, P.; Goud, E. V.; Pavankumar, B. B.; Leninkumar, V.; Bhat, H. R.; Sivaramakrishna, A.; Vijayakrishna, K.; Jha, P. C.; Smith, G. S.

Synthesis, structure and thermolysis of cis-dialkylplatinum(II) complexes - Experimental and theoretical perceptions
Journal of Organometallic Chemistry, (818): 72-81. 2016. 10.1016/j.jorgchem.2016.05.023

Vent-Schmidt, T.; Fang, Z. T.; Lee, Z.; Dixon, D.; Riedel, S.

Extending the Row of Lanthanide Tetrafluorides: A Combined Matrix-Isolation and Quantum-Chemical Study
Chemistry-a European Journal, (22): 2406-2416. 2016. 10.1002/chem.201504182

Vepuri, S. B.; Devarajegowda, H. C.; Soliman, M. E.

Synthesis, characterization and molecular modelling of a novel dipyridamole supramolecule - X-ray structure, quantum mechanics and molecular dynamics study to comprehend the hydrogen bond structure-activity relationship
Journal of Molecular Structure, (1105): 194-204. 2016. 10.1016/j.molstruc.2015.10.050

Verma, A. K.; Bishnoi, A.; Fatma, S.

Synthesis, spectral analysis and quantum chemical studies on molecular geometry of (2E,6E)-2,6-bis(2-chlorobenzylidene) cyclohexanone: Experimental and theoretical approaches
Journal of Molecular Structure, (1116): 9-21. 2016. 10.1016/j.molstruc.2016.02.077

Verma, M.; Deshpande, P. A.

Computational Design of New Heterofullerene-Based Biomimetic alpha-Carbonic Anhydrase Analogues
Chemphyschem, (17): 3120-3128. 2016. 10.1002/cphc.201600649

Verma, P.; Derricotte, W. D.; Evangelista, F. A.

Predicting Near Edge X-ray Absorption Spectra with the Spin-Free Exact-Two-Component Hamiltonian and Orthogonality Constrained Density Functional Theory
Journal of Chemical Theory and Computation, (12): 144-156. 2016. 10.1021/acs.jctc.5b00817

Verma, P. L.; Bartolotti, L. J.; Gejji, S. P.

Probing Molecular Interactions in Functionalized Asymmetric Quaternary Ammonium-Based Dicationic Ionic Liquids
Journal of Physical Chemistry A, (120): 7732-7744. 2016. 10.1021/acs.jpca.6b07337

Verstraelen, T.; Vandenbrande, S.; Heidar-Zadeh, F.; Vanduyfhuys, L.; Van Speybroeck, V.; Waroquier, M.; Ayers, P. W.

Minimal Basis Iterative Stockholder: Atoms in Molecules for Force-Field Development

Journal of Chemical Theory and Computation, (12): 3894-3912. 2016. 10.1021/acs.jctc.6b00456

Vessally, E.; Behmaghan, F.; Massoumi, B.; Hosseiniyan, A.; Edjlali, L.

Carbon nanocone as an electronic sensor for HCl gas: Quantum chemical analysis
Vacuum, (134): 40-47. 2016. 10.1016/j.vacuum.2016.09.019

Viana, R. B.

Tailoring the electronic properties among oxoarsine, arsinoyl and arsine oxide isomers: the simplest molecular systems with an arsenic-oxygen bond

- Viana, R. B.; Ribeiro, G. L. O.; Santos, S. F. F.; Quintero, D. E.; Viana, A. B.; da Silva, A. B. F.; Moreno-Fuquen, R.
Intramolecular interactions, isomerization and vibrational frequencies of two paracetamol analogues: A spectroscopic and a computational approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (162): 16-26. 2016. 10.1016/j.saa.2016.02.037
- Viana, R. B.; Ribeiro, G. L. O.; Valencia, L. J.; Varela, J. J. G.; Viana, A. B.; da Silva, A. B. F.; Moreno-Fuquen, R.
Vibrational spectroscopy, intramolecular CH center dot center dot center dot O interaction and conformational analysis of 2,5-dimethyl-benzyl benzoate
Journal of Molecular Structure, (1125): 649-655. 2016. 10.1016/j.molstruc.2016.07.041
- Viana, R. B.; Varela, J. J. G.; Tello, A. C. M.; Savedra, R. M. L.; da Silva, A. B. F.
The 1,2-hydrogen shift reaction for monohalogenophosphanes PH₂X and HPX (X = F, Cl)
Molecular Physics, (114): 2999-3014. 2016. 10.1080/00268976.2016.1213438
- Vicha, J.; Marek, R.; Straka, M.
High-Frequency C-13 and Si-29 NMR Chemical Shifts in Diamagnetic Low-Valence Compounds of Tl^{II} and Pb^{II}: Decisive Role of Relativistic Effects
Inorganic Chemistry, (55): 1770-1781. 2016. 10.1021/acs.inorgchem.5b02689
- Vicha, J.; Marek, R.; Straka, M.
High-Frequency H-1 NMR Chemical Shifts of Sn-II and Pb-II Hydrides Induced by Relativistic Effects: Quest for Pb-II Hydrides
Inorganic Chemistry, (55): 10302-10309. 2016. 10.1021/acs.inorgchem.6b01575
- Vidhani, D. V.; Krafft, M. E.; Alabugin, I. V.
Gold(I)-Catalyzed Allenyl Cope Rearrangement: Evolution from Asynchronicity to Trappable Intermediates Assisted by Stereoelectronic Switching
Journal of the American Chemical Society, (138): 2769-2779. 2016. 10.1021/jacs.5b12920
- Viesser, R. V.; Ducati, L. C.; Autschbach, J.; Tormena, C. F.
NMR spin-spin coupling constants: bond angle dependence of the sign and magnitude of the vicinal (3)J(HF) coupling
Physical Chemistry Chemical Physics, (18): 24119-24128. 2016. 10.1039/c6cp04853f
- Vijayalakshmi, S.; Kalyanaraman, S.
Role of charge transfer on the nonlinear optical properties of donor-acceptor (D-a) conjugated schiffbases with DFT approach
Journal of Physical Organic Chemistry, (29): 436-442. 2016. 10.1002/poc.3556
- Vijayan, P.; Viswanathanurthi, P.; Sugumar, P.; PonnuSwamy, M. N.; Velmurugan, K.; Nandhakumar, R.; Balakumaran, M. D.; KalaiChelvan, P. T.
Toward a new avenue in ruthenium-sulphur chemistry of binuclear mu-sulphido bridged (mu-S)(2) complexes having Ru2S2 core: Targeted synthesis, crystal structure, biomolecules interaction and their in vitro anticancer activities
Inorganica Chimica Acta, (453): 596-617. 2016. 10.1016/j.ica.2016.09.024
- Vinod, K. S.; Periandy, S.; Govindarajan, M.
Spectroscopic FT-IR and FT-Raman and molecular modeling (MM) study of benzene sulfonamide molecule using quantum chemical calculations
Journal of Molecular Structure, (1116): 226-235. 2016. 10.1016/j.molstruc.2016.03.024
- Vishwakarma, P. K.; Mir, J. M.; Maurya, R. C.
Pyrone-based Cu(II) complexes, their characterization, DFT based conformational drift from square planar to square pyramidal geometry and biological activities
Journal of Chemical Sciences, (128): 511-522. 2016. 10.1007/s12039-016-1048-6
- Visscher, A.; Bachmann, S.; Schnegelsberg, C.; Teuteberg, T.; Mata, R. A.; Stalke, D.
Highly selective and sensitive fluorescence detection of Zn²⁺ and Cd²⁺ ions by using an acridine sensor

Dalton Transactions, (45): 5689-5699. 2016. 10.1039/c6dt00557h

Vogt, N.; Savelyev, D. S.; Giricheva, N. I.; Islyaikin, M. K.; Girichev, G. V.

Accurate Determination of Equilibrium Structure of 3-Aminophthalonitrile by Gas Electron Diffraction and Coupled-Cluster Computations: Structural Effects Due to Intramolecular Charge Transfer
Journal of Physical Chemistry A, (120): 8853-8861. 2016. 10.1021/acs.jpca.6b08241

Vogt-Geisse, S.; Toro-Labbe, A.

Chemical potential and reaction electronic flux in symmetry controlled reactions
Journal of Computational Chemistry, (37): 1794-1800. 2016. 10.1002/jcc.24394

von Szentpaly, L.

Comment on "A new equation based on ionization energies and electron affinities of atoms for calculating of group electronegativity" by S. Kaya and C. Kaya Comput. Theoret. Chem. 1052 (2015) 42-46
Computational and Theoretical Chemistry, (1083): 72-74. 2016. 10.1016/j.comptc.2016.02.008

von Wolff, N.; Lefevre, G.; Berthet, J. C.; Thuery, P.; Cantat, T.

Implications of CO₂ Activation by Frustrated Lewis Pairs in the Catalytic Hydroboration of CO₂: A View Using N/Si+ Frustrated Lewis Pairs
ACS Catalysis, (6): 4526-4535. 2016. 10.1021/acscatal.6b00421

Vrana, J.; Ketkov, S.; Jambor, R.; Ruzicka, A.; Lycka, A.; Dostal, L.

Germylenes and stannylenes stabilized within N₂PE rings (E = Ge or Sn): combined experimental and theoretical study
Dalton Transactions, (45): 10343-10354. 2016. 10.1039/c6dt01616b

Vranova, I.; Alonso, M.; Jambor, R.; Ruzicka, A.; Erben, M.; Dostal, L.

Stibinidene and Bismuthinidene as Two-Electron Donors for Transition Metals (Co and Mn)
Chemistry-a European Journal, (22): 7376-7380. 2016. 10.1002/chem.201601272

Vural, H.

Experimental and computational studies of 4-(Trifluoromethyl)pyridine-2-carboxylic acid
Journal of Molecular Structure, (1111): 55-60. 2016. 10.1016/j.molstruc.2016.01.076

Vural, H.; Kara, M.; Idil, O.

Experimental and computational study of the structure and spectroscopic properties of 1',3'-Dihydrospiro cyclohexane-1,2'-2H imidazo 4,5-b pyridine
Journal of Molecular Structure, (1125): 662-670. 2016. 10.1016/j.molstruc.2016.07.065

Vural, H.; Ucar, I.

A mixed experimental and theoretical study on chelidamate copper(II) complex with 4-methylpyrimidine
Journal of Coordination Chemistry, (69): 3010-3020. 2016. 10.1080/00958972.2016.1225042

Vural, H.; Ucar, I.; Soylu, M. S.

Combined experimental-theoretical characterization of chelidamate nickel complex with 4-methylpyrimidine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (152): 584-590. 2016.
10.1016/j.saa.2014.12.118

Vyas, V. K.; Bhanage, B. M.

Asymmetric transfer hydrogenation of seven membered tricyclic ketones: N-substituted dibenzo b,e azepine-6,11-dione driven by nonclassical CH/O interactions
Organic Chemistry Frontiers, (3): 614-619. 2016. 10.1039/c6qo00036c

Wahab, A.; Kaleta, J.; Wen, J.; Valasek, M.; Polasek, M.; Michl, J.; Ludvik, J.

Electrochemical Oxidation of 1-X-12-I-CB11Me10- Anions: Formation of Borenium Ylides 12-Dehydro-1-X-CB11Me10 and Iodonium Ylide Anions {12-(1-X-CB11Me10-)}(2)I+
Inorganic Chemistry, (55): 12815-12821. 2016. 10.1021/acs.inorgchem.6b02128

Wandtke, C. M.; Lubben, J.; Dittrich, B.

Molecular Electrostatic Potentials from Invariom Point Charges
Chemphyschem, (17): 2238-2246. 2016. 10.1002/cphc.201600213

Wang, B.; Jiang, W. R.; Dai, X.; Gao, Y.; Wang, Z. G.; Zhang, R. Q.
Molecular orbital analysis of the hydrogen bonded water dimer
Scientific Reports, (6) 2016. 10.1038/srep22099

Wang, B. F.; Wen, X.; Xi, Z.
Molecular Simulations Bring New Insights into Protoporphyrinogen IX Oxidase/Protoporphyrinogen IX Interaction Modes
Molecular Informatics, (35): 476-482. 2016. 10.1002/minf.201600008

Wang, C. W.; Guan, L. Y.; Danovich, D.; Shaik, S.; Mo, Y. R.
The Origins of the Directionality of Noncovalent Intermolecular Interactions
Journal of Computational Chemistry, (37): 34-45. 2016. 10.1002/jcc.23946

Wang, D. Y.; Choliy, Y.; Haibach, M. C.; Hartwig, J. F.; Krogh-Jespersen, K.; Goldman, A. S.
Assessment of the Electronic Factors Determining the Thermodynamics of "Oxidative Addition" of C-H and N-H Bonds to Ir(I) Complexes
Journal of the American Chemical Society, (138): 149-163. 2016. 10.1021/jacs.5b09522

Wang, G. M.; Chen, Z. Q.; Xu, Z. J.; Wang, J. N.; Yang, Y.; Cai, T. T.; Shi, J. Y.; Zhu, W. L.
Stability and Characteristics of the Halogen Bonding Interaction in an Anion-Anion Complex: A Computational Chemistry Study
Journal of Physical Chemistry B, (120): 610-620. 2016. 10.1021/acs.jpcb.5b08139

Wang, H.; Cheng, Y.; Becker, P.; Raabe, G.; Bolm, C.
Synthesis of Sulfoximidoyl-Containing Hypervalent Iodine(III) Reagents and Their Use in Transition-Metal-Free Sulfoximidations of Alkynes
Angewandte Chemie-International Edition, (55): 12655-12658. 2016. 10.1002/anie.201605743

Wang, H. B.; Shi, W. J.; Ren, F. D.; Tan, Y. X.
Does HF prefer to be attached to X or M of XHHM (X = F, Cl, Br; M = Li, Na, K) system? A B3LYP and MP2 theoretical investigation into cooperativity effect
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (55): 769-781. 2016.

Wang, H. Y.; Wang, H.; King, R. B.; Schaefer, H. F.
Bis(azulene) "Submarine" Metal Dimer Sandwich Compounds ($C_{10}H_8(2)M-2$ (M = Ti, V, Cr, Mn, Fe, Co, Ni): Parallel and Opposed Orientations
Journal of Computational Chemistry, (37): 250-260. 2016. 10.1002/jcc.24013

Wang, H. Z.; Huang, J.; Zhang, S. Y.; Xu, Y.; Zhang, K. L.; Liu, K.; Cao, Z. G.; Yu, G.; Deng, S. B.; Wang, Y. J.; Wang, B.
Study of degradation mechanism of dechlorane plus by mechanochemical reaction with aluminum and quartz sand
Chemical Engineering Journal, (292): 98-104. 2016. 10.1016/j.cej.2016.02.011

Wang, J.; Liu, Y.
New Volleyballenes: Y₂₀C₆₀ and La₂₀C₆₀
Scientific Reports, (6) 2016. 10.1038/srep30875

Wang, J.; Ma, H. M.; Liu, Y.
Sc₂₀C₆₀: a volleyballene
Nanoscale, (8): 11441-11444. 2016. 10.1039/c5nr07784b

Wang, J. M.; Su, Z. S.; Yang, N.; Hu, C. W.
Mechanistic Study of the Asymmetric Carbonyl-Ene Reaction between Alkyl Enol Ethers and Isatin Catalyzed by the N,N'-Dioxide-Mg(OTf)₂ Complex
Journal of Organic Chemistry, (81): 6444-6456. 2016. 10.1021/acs.joc.6b01071

- Wang, K.; Chen, J. G.; Wang, B. Z.; Ji, Y. P.; Liu, F. Y.; Liu, Z. T.; Wang, W. L.; Liu, Z. W.; Hao, Z. P.; Lu, J.
Insight into the acidic group-induced nitration mechanism of 2-methyl-4,6-dihydroxypyrimidine (MDP) with nitronium
RSC Advances, (6): 80145-80157. 2016. 10.1039/c6ra18842g
- Wang, K.; Li, D. Z.; Li, R.; Feng, L. Y.; Wang, Y. J.; Zhai, H. J.
Concentric dual pi aromaticity in bowl-like B-30 cluster: an all-boron analogue of corannulene
Physical Chemistry Chemical Physics, (18): 23304-23311. 2016. 10.1039/c6cp04464f
- Wang, K.; Wang, Y. J.; Li, D. Z.; Ou, T.; Zhao, X. Y.; Zhai, H. J.
On the nature of bonding in binary Be₂O₂ and Si₂O₂ clusters: rhombic four-center four-electron pi and sigma bonds
Physical Chemistry Chemical Physics, (18): 9594-9601. 2016. 10.1039/c6cp00532b
- Wang, L. S.
Photoelectron spectroscopy of size-selected boron clusters: from planar structures to borophenes and borospherenes
International Reviews in Physical Chemistry, (35): 69-142. 2016. 10.1080/0144235x.2016.1147816
- Wang, N.; Zheng, S. C.; Zhang, L. L.; Guo, Z.; Liu, X. Y.
Nickel(0)-Catalyzed Denitrogenative Transannulation of Benzotriazinones with Alkynes: Mechanistic Insights of Chemical Reactivity and Regio- and Enantioselectivity from Density Functional Theory and Experiment
ACS Catalysis, (6): 3496-3505. 2016. 10.1021/acscatal.6b00572
- Wang, Q. Q.; Li, P.; Gao, T.; Ao, B. Y.
Mechanistic aspects of the activation of C-H bond in C₂H₆ by Th atom: bonding analysis and reaction coefficients
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-2015-5
- Wang, Q. W.; Sui, W.; Wang, Y. N.; Li, X. M.; Liu, B.
Syntheses, Crystal Structures and Theoretical Calculations of Nickel/Cobalt Supramolecular Coordination Compounds
Chinese Journal of Inorganic Chemistry, (32): 1120-1126. 2016. 10.11862/cjic.2016.133
- Wang, Q. Y.; Tong, Y. C.; Xu, X. J.; Wang, Y. C.
Theoretical study on the H₂S activation by PtCH₂ (+) in the gas phase
Structural Chemistry, (27): 1363-1371. 2016. 10.1007/s11224-016-0756-3
- Wang, S. H.; Fang, W. H.; Li, T. Y.; Li, F. F.; Sun, C. L.; Li, Z. W.; Huang, Y. X.; Men, Z. W.
An insight into liquid water networks through hydrogen bonding halide anion: Stimulated Raman scattering
Journal of Applied Physics, (119) 2016. 10.1063/1.4947292
- Wang, S. S.; Zhao, P. W.; Zhang, C. Z.; Bu, Y. X.
The Equally Important Role of Adenine Derivatives to That of Pyrimidine Derivatives in Near-0 eV Electron-Induced DNA Lesions
Chemphyschem, (17): 1669-1677. 2016. 10.1002/cphc.201600002
- Wang, T.; Ge, K.; Chen, K. X.; Hou, C. L.; Fang, M. X.
Theoretical studies on CO₂ capture behavior of quaternary ammonium-based polymeric ionic liquids
Physical Chemistry Chemical Physics, (18): 13084-13091. 2016. 10.1039/c5cp07229h
- Wang, W.; Mao, S.; Peng, D.; Li, L. C.
Investigation on the Mechanism for N-Methylindole and Keto Ester Catalyzed by InX₃ (X=F, Br)
Chinese Journal of Organic Chemistry, (36): 613-621. 2016. 10.6023/cjoc201508026
- Wang, W. J.; Sheng, X. H.; Zhang, S. L.; Huang, F.; Sun, C. Z.; Liu, J. B.; Chen, D. Z.
Theoretical characterization of the conformational features of unnatural oligonucleotides containing a six nucleotide genetic alphabet
Physical Chemistry Chemical Physics, (18): 28492-28501. 2016. 10.1039/c6cp05594j
- Wang, X.; Bai, F. Y.; Sun, Y. Q.; Wang, R. S.; Pan, X. M.; Tao, F. M.
Theoretical study of the gaseous hydrolysis of NO₂ in the presence of NH₃ as a source of atmospheric HONO

Environmental Chemistry, (13): 611-622. 2016. 10.1071/en15076

Wang, X. J.; Zhao, Y.; Li, F. T.; Dou, L. J.; Li, Y. P.; Zhao, J.; Hao, Y. J.

A Chelation Strategy for In-situ Constructing Surface Oxygen Vacancy on {001} Facets Exposed BiOBr Nanosheets
Scientific Reports, (6) 2016. 10.1038/srep24918

Wang, X. L.; Wang, Y. C.; Li, S.; Zhang, Y. W.; Ma, P. P.

Theoretical Study on the Reaction Mechanism of Ti with CH₃CN in the Gas Phase
Journal of Physical Chemistry A, (120): 5457-5463. 2016. 10.1021/acs.jpca.6b04733

Wang, Y.; Tang, M. S.; Wang, Y. Y.; Wei, D. H.

Insights into Stereoselective Aminomethylation Reaction of alpha,beta-Unsaturated Aldehyde with N,O-Acetal via N-Heterocyclic Carbene and Bronsted Acid/Base Cooperative Organocatalysis
Journal of Organic Chemistry, (81): 5370-5380. 2016. 10.1021/acs.joc.6b00656

Wang, Y.; Wu, B. H.; Zhang, H. Y.; Wei, D. H.; Tang, M. S.

A computational study on the N-heterocyclic carbene-catalyzed C-sp₂-C-sp₃ bond activation/4+2 cycloaddition cascade reaction of cyclobutenones with imines: a new application of the conservation principle of molecular orbital symmetry
Physical Chemistry Chemical Physics, (18): 19933-19943. 2016. 10.1039/c6cp03180c

Wang, Y.; Wu, B. H.; Zheng, L. J.; Wei, D. H.; Tang, M. S.

DFT perspective toward 3+2 annulation reaction of enals with alpha-ketoamides through NHC and Bronsted acid cooperative catalysis: mechanism, stereoselectivity, and role of NHC
Organic Chemistry Frontiers, (3): 190-203. 2016. 10.1039/c5qo00338e

Wang, Y. H.; Li, X. Y.; Zeng, Y. L.; Meng, L. P.; Zhang, X. Y.

Topological Analyses of Electron Density on pi-hole Pnicogen Bonds in PO₂X center dot center dot center dot center dot PX₃/PH₂X (X = F, Cl, Br, CH₃, NH₂) Complexes
Acta Physico-Chimica Sinica, (32): 671-682. 2016. 10.3866/pku.Whxb201512293

Wang, Y. L.; Wang, Y.; Yi, H. B.

High-Order Ca(II)-Chloro Complexes in Mixed CaCl₂-LiCl Aqueous Solution: Insights from Density Functional Theory and Molecular Dynamics Simulations
Journal of Physical Chemistry A, (120): 5635-5648. 2016. 10.1021/acs.jpca.6b01694

Wang, Y. P.; Zhang, Z. X.; Xie, M.; Bai, F. Q.; Wang, P. X.; Zhang, H. X.

Theoretical study on thermal cis-to-trans isomerization of BF₂-coordinated azo compounds of the para-substitution with electron donating groups
Dyes and Pigments, (129): 100-108. 2016. 10.1016/j.dyepig.2016.02.025

Wang, Y. X.; Zheng, W. R.; Ding, L. L.

The C-H bond dissociation enthalpies in fused N-heterocyclic compounds
Russian Journal of Physical Chemistry A, (90): 610-621. 2016. 10.1134/s0036024416030353

Wang, Y. Y.; Wei, D. H.; Wang, Y.; Zhang, W. J.; Tang, M. S.

N-Heterocyclic Carbene (NHC)-Catalyzed sp(3) beta-C-H Activation of Saturated Carbonyl Compounds: Mechanism, Role of NHC, and Origin of Stereoselectivity
ACS Catalysis, (6): 279-289. 2016. 10.1021/acscatal.5b01710

Wannakao, S.; Maihom, T.; Probst, M.; Limtrakul, J.; Kongpatpanich, K.

Porous Materials as a Platform for Highly Uniform Single-Atom Catalysts: Tuning the Electronic Structure for the Low-Temperature Oxidation of Carbon Monoxide
Journal of Physical Chemistry C, (120): 19686-19697. 2016. 10.1021/acs.jpcc.6b05205

Wazzan, N. A.; Obot, I. B.; Kaya, S.

Theoretical modeling and molecular level insights into the corrosion inhibition activity of 2-amino-1,3,4-thiadiazole and its 5-alkyl derivatives

Journal of Molecular Liquids, (221): 579-602. 2016. 10.1016/j.molliq.2016.06.011

Webster, A. J.; Mueller, C. M.; Foegen, N. P.; Sit, P. H. L.; Speetzen, E. D.; Cunningham, D. W.; D'Acchioli, J. S.
Oxidation states "naturally": A Natural Bond Orbital method for determining transition metal oxidation states
Polyhedron, (114): 128-132. 2016. 10.1016/j.poly.2015.11.018

Wei, Q. C.; Li, Q. Z.; Cheng, J. B.; Li, W. Z.; Li, H. B.
Comparison of tetrel bonds and halogen bonds in complexes of DMSO with ZF(3)X (Z = C and Si; X = halogen)
RSC Advances, (6): 79245-79253. 2016. 10.1039/c6ra18316f

Wei, Y. X.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.; McDowell, S. A. C.
Influence of the protonation of pyridine nitrogen on pnictogen bonding: competition and cooperativity
Physical Chemistry Chemical Physics, (18): 11348-11356. 2016. 10.1039/c6cp00551a

Weinhold, F.; Landis, C. R.; Glendening, E. D.
What is NBO analysis and how is it useful?
International Reviews in Physical Chemistry, (35): 399-440. 2016. 10.1080/0144235x.2016.1192262

Weismann, J.; Waterman, R.; Gessner, V. H.
Metal-Ligand Cooperativity in a Methandiide-Derived Iridium Carbene Complex
Chemistry-a European Journal, (22): 3846-3855. 2016. 10.1002/chem.201503936

Weiss, N. M.; Waller, A. W.; Phillips, J. A.
Infrared spectrum of CH₃CN-HCl in solid neon, and modeling matrix effects in CH₃CN-HCl and H₃N-HCl
Journal of Molecular Structure, (1105): 341-349. 2016. 10.1016/j.molstruc.2015.10.014

Wentrup, C.; Koch, R.; Kleinpeter, E.
Twisted C=C Double Bonds with Very Low Rotational Barriers in Dioxanediones and Isoxazolones Determined by Low-Temperature Dynamic NMR Spectroscopy and Computational Chemistry
European Journal of Organic Chemistry: 4985-4990. 2016. 10.1002/ejoc.201600931

Werle, C.; Anstine, D. M.; Karmazin, L.; Bailly, C.; Ricard, L.; Djukic, J. P.
New Pd(II) hemichelates devoid of incipient bridging CO center dot center dot center dot center dot Pd interactions
Dalton Transactions, (45): 607-617. 2016. 10.1039/c5dt03648h

Wern, M.; Hoppe, T.; Becker, J.; Zahn, S.; Mollenhauer, D.; Schindler, S.
Sulfur versus Dioxygen: Dinuclear (Trisulfido)copper Complexes
European Journal of Inorganic Chemistry: 3384-3388. 2016. 10.1002/ejic.201600614

West, C. W.; Bull, J. N.; Woods, D. A.; Verlet, J. R. R.
Photoelectron imaging as a probe of the repulsive Coulomb barrier in the photodetachment of antimony tartrate dianions
Chemical Physics Letters, (645): 138-143. 2016. 10.1016/j.cplett.2015.12.041

Weston, L.; Pownall, B. T.; Mair, F. S.; McDouall, J. J. W.
Thalophilic Tl(I)-Tl(I) contacts mediated by Tl-aryl interactions. A computational study
Dalton Transactions, (45): 8433-8439. 2016. 10.1039/c6dt01035k

Wiberg, K. B.; Frisch, M. J.
Effect of Conjugation on Electron Distributions. Separation of sigma and pi Terms
Journal of Chemical Theory and Computation, (12): 1220-1227. 2016. 10.1021/acs.jctc.5b01149

Wierzejewska, M.; Yaremko, A. M.; Virko, S. V.; Barnes, A. J.; Ratajczak, H.
On the unusual IR spectra of the pentachlorophenol - Trimethylamine complex in low temperature matrices
Chemical Physics Letters, (660): 102-106. 2016. 10.1016/j.cplett.2016.07.052

Wildman, E. P.; Balazs, G.; Woole, A. J.; Scheer, M.; Liddle, S. T.
Thorium-phosphorus triamidoamine complexes containing Th-P single- and multiple-bond interactions

Nature Communications, (7) 2016. 10.1038/ncomms12884

Wilke, J.; Wilke, M.; Brand, C.; Meerts, W. L.; Schmitt, M.

On the Additivity of Molecular Fragment Dipole Moments of 5-Substituted Indole Derivatives
Chemphyschem, (17): 2736-2743. 2016. 10.1002/cphc.201600420

Wilke, J.; Wilke, M.; Meerts, W. L.; Schmitt, M.

Determination of ground and excited state dipole moments via electronic Stark spectroscopy: 5-methoxyindole
Journal of Chemical Physics, (144) 2016. 10.1063/1.4940689

Wilke, M.; Brand, C.; Wilke, J.; Schmitt, M.

The conformational space of the neurotransmitter serotonin: how the rotation of a hydroxyl group changes all
Physical Chemistry Chemical Physics, (18): 13538-13545. 2016. 10.1039/c6cp02130a

Winston, M. S.; Batista, E. R.; Yang, P.; Tondreau, A. M.; Boncella, J. M.

Extending Stannyli Anion Chemistry to the Actinides: Synthesis and Characterization of a Uranium-Tin Bond
Inorganic Chemistry, (55): 5534-5539. 2016. 10.1021/acs.inorgchem.6b00543

Witteman, L.; Evers, T.; Shu, Z.; Lutz, M.; Gebbink, R.; Moret, M. E.

Hydrosilylation in Aryliminopyrrolide-Substituted Silanes
Chemistry-a European Journal, (22): 6087-6099. 2016. 10.1002/chem.201505033

Wojciechowska, A.; Kochel, A.; Zierkiewicz, W.

1-D Framework L-arginine zinc(II) units bridged by oxalate: synthesis, structure, properties, and theoretical studies
Journal of Coordination Chemistry, (69): 886-900. 2016. 10.1080/00958972.2016.1147561

Wong, Z. X.; Lein, M.

Guest-Host Interaction of Coinage Metals in pi-Rich Cavities
Australian Journal of Chemistry, (69): 969-974. 2016. 10.1071/ch16208

Word, T. A.; Karolak, A.; Cioce, C. R.; Van Der Vaart, A.; Larsen, R. W.

Using Photoacoustic Calorimetry to Study the cis- to trans-Photoisomerization of the Ru(II)(2,2'-bipyridine)(2)(H₂O)(2)(2+)-Complex in Aqueous Solution
Comments on Inorganic Chemistry, (36): 343-354. 2016. 10.1080/02603594.2016.1183488

Wrobel, A. J.; Lucchesi, R.; Wibbeling, B.; Daniliuc, C. G.; Frohlich, R.; Wurthwein, E. U.

1,3,5-Triazapentadienes by Nucleophilic Addition to 1,3-and 1,4-Dinitriles-Sterically Constrained Examples by Incorporation into Cyclic Peripheries: Synthesis, Aggregation, and Photophysical Properties
Journal of Organic Chemistry, (81): 2849-2863. 2016. 10.1021/acs.joc.6b00126

Wu, D. L.; Jiang, W.; Liu, X. Q.; Qiu, N. X.; Xue, Y.

Theoretical Study About Effects of H₂O and Na⁺ on Adsorption of CO₂ on Kaolinite Surfaces
Chemical Research in Chinese Universities, (32): 118-126. 2016. 10.1007/s40242-016-5201-z

Wu, J.; Kucukkal, M. U.; Clark, A. E.

H-2 Adsorbed Site-to-Site Electronic Delocalization within IRMOF-1: Understanding Non-Negligible Interactions at High Pressure
Materials, (9) 2016. 10.3390/ma9070578

Wu, Q. Y.; Zhai, F. W.; Liu, Y.; Yuan, L. Y.; Chai, Z. F.; Shi, W. Q.

Interactions between uranium(VI) and phosphopeptide: experimental and theoretical investigations
Dalton Transactions, (45): 14988-14997. 2016. 10.1039/c6dt03009b

Wyss, C. M.; Bitting, J.; Bacsa, J.; Gray, T. G.; Sadighi, J. P.

Bonding and Reactivity of a Dicopper(I) mu-Boryl Cation
Organometallics, (35): 71-74. 2016. 10.1021/acs.organomet.5b00961

Xavier, S.; Periandy, S.; Carthigayan, K.; Sebastian, S.

Molecular docking, TG/DTA, molecular structure, harmonic vibrational frequencies, natural bond orbital and TD-DFT analysis of diphenyl carbonate by DFT approach
Journal of Molecular Structure, (1125): 204-216. 2016. 10.1016/j.molstruc.2016.06.071

Xia, J. J.; Wu, P.
A computational study on the thermal decomposition of di(tri)thiocarbonates
Journal of Theoretical & Computational Chemistry, (15) 2016. 10.1142/s0219633616500619

Xiao-Hong, L.; Zheng, M.; Rui-Zhou, Z.; Xian-Zhou, Z.
Theoretical investigation of a series of bis(1H-tetrazol-5-yl)furan and bis(1H-tetrazol) derivatives as high-energy-density materials
Molecular Physics, (114): 3437-3447. 2016. 10.1080/00268976.2016.1235287

Xie, F. K.; Du, C.; Pang, Y. D.; Lian, X.; Xue, C. T.; Chen, Y. Y.; Wang, X. F.; Cheng, M. S.; Guo, C.; Lin, B.; Liu, Y. X.
Lewis acid-assisted N-fluorobenzenesulfonimide-based electrophilic fluorine catalysis in Beckmann rearrangement
Tetrahedron Letters, (57): 5820-5824. 2016. 10.1016/j.tetlet.2016.11.054

Xie, H. J.; Li, Y.; Huang, L. T.; Nong, F. L.; Ren, G. R.; Fan, T.; Lei, Q. F.; Fang, W.
Dehydrogenation of benzyl alcohol with N₂O as the hydrogen acceptor catalyzed by the rhodium(I) carbene complex: insights from quantum chemistry calculations
Dalton Transactions, (45): 16485-16491. 2016. 10.1039/c6dt02900k

Xie, H. J.; Liu, C. C.; Yuan, Y.; Zhou, T.; Fan, T.; Lei, Q. F.; Fang, W. J.
Oxidation of phenyl and hydride ligands of bis(pentamethylcyclopentadienyl) hafnium derivatives by nitrous oxide via selective oxygen atom transfer reactions: insights from quantum chemistry calculations
Dalton Transactions, (45): 1152-1159. 2016. 10.1039/c5dt03264d

Xie, J.; Zuo, T. F.; Huang, Z. L.; Huan, L.; Gu, Q. X.; Gao, C. X.; Shao, J. J.
Theoretical study of a novel imino bridged pillar 5 arene derivative
Chemical Physics Letters, (662): 25-30. 2016. 10.1016/j.cplett.2016.09.010

Xie, L.; Zhao, Q.; Jensen, K. F.; Kulik, H. J.
Direct Observation of Early-Stage Quantum Dot Growth Mechanisms with High-Temperature Ab Initio Molecular Dynamics
Journal of Physical Chemistry C, (120): 2472-2483. 2016. 10.1021/acs.jpcc.5b12091

Xie, L. H.; Huang, F.; Sun, C. Z.; Liu, J. B.; Chen, D. Z.
Mechanistic insight into the prebiotic syntheses of pyrimidine ribonucleotide and pyrimidine deoxynucleotide precursors
Computational and Theoretical Chemistry, (1079): 11-22. 2016. 10.1016/j.comptc.2016.01.006

Xie, M.; Matsuda, Y.; Fujii, A.
Infrared Spectroscopic Investigation of the Acidic CH Bonds in Cationic n-Alkanes: Pentane, Hexane, and Heptane
Journal of Physical Chemistry A, (120): 6351-6356. 2016. 10.1021/acs.jpca.6b05567

Xing, Y. X.; Jindal, A. K.; Regueiro-Figueroa, M.; Le Fur, M.; Kervarec, N.; Zhao, P. Y.; Kovacs, Z.; Valencia, L.; Perez-Lourido, P.; Tripier, R.; Esteban-Gomez, D.; Platas-Iglesias, C.; Sherry, A. D.
The Relationship between NMR Chemical Shifts of Thermally Polarized and Hyperpolarized Y-89 Complexes and Their Solution Structures
Chemistry-a European Journal, (22): 16657-16667. 2016. 10.1002/chem.201602901

Xing, Y. Y.; Liu, J. B.; Tian, Y. Y.; Sun, C. Z.; Huang, F.; Chen, D. Z.
Computational Mechanistic Study of Redox-Neutral Rh(III)-Catalyzed C-H Activation Reactions of Arylnitrones with Alkynes: Role of Noncovalent Interactions in Controlling Selectivity
Journal of Physical Chemistry A, (120): 9151-9158. 2016. 10.1021/acs.jpca.6610367

Xu, B.; Li, Q. S.; Xie, Y. M.; King, R. B.
Binuclear rhenium carbonyl nitrosyls related to dicobalt octacarbonyl and their decarbonylation products

Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3028-7

Xu, C. Q.; Xiong, X. G.; Li, W. L.; Li, J.

Periodicity and Covalency of MX₂ (-) (M = Cu, Ag, Au, Rg; X = H, Cl, CN) Complexes

European Journal of Inorganic Chemistry: 1395-1404. 2016. 10.1002/ejic.201600002

Xu, H. L.; Cheng, J. B.; Li, Q. Z.; Li, W. Z.

Some measures for making a traditional halogen bond be chlorine-shared or ion-pair one in FCl center dot NH₃ complex

Molecular Physics, (114): 3643-3649. 2016. 10.1080/00268976.2016.1255798

Xu, H. Y.; Zhang, X. P.; Ke, Z. F.; Zhao, C. Y.

A theoretical study of dirhodium-catalyzed intramolecular aliphatic C-H bond amination of aryl azides

RSC Advances, (6): 29045-29053. 2016. 10.1039/c5ra24340h

Xu, L. P.; Chung, L. W.; Wu, Y. D.

Mechanism of Ni-NHC Catalyzed Hydrogenolysis of Aryl Ethers: Roles of the Excess Base

ACS Catalysis, (6): 483-493. 2016. 10.1021/acscatal.5b02089

Xu, P. L.; Zhou, T.; Natalia, N.; Hu, S. J.; Zheng, X.

Rational Ligand Design for an Efficient Biomimetic Water Splitting Complex

Journal of Physical Chemistry A, (120): 10033-10042. 2016. 10.1021/acs.jpca.6b10154

Xu, Q.; Liu, H. X.; Song, Z.; Huang, X. C.; Ullah, A.; Zhang, L.; Xie, J.; Hao, H.; Cao, M. H.; Yao, Z. H.

A new energy-storage ceramic system based on Bi0.5Na0.5TiO3 ternary solid solution

Journal of Materials Science-Materials in Electronics, (27): 322-329. 2016. 10.1007/s10854-015-3757-x

Xu, S.; Smith, J. E. T.; Weber, J. M.

Ligand Influence on the Electronic Spectra of Dicationic Ruthenium-Bipyridine-Terpyridine Complexes

Journal of Physical Chemistry A, (120): 2350-2356. 2016. 10.1021/acs.jpca.6b02926

Xu, S.; Smith, J. E. T.; Weber, J. M.

UV Spectra of Tris(2,2'-bipyridine) M(II) Complex Ions in Vacuo (M = Mn, Fe, Co, Ni, Cu, Zn)

Inorganic Chemistry, (55): 11937-11943. 2016. 10.1021/acs.inorgchem.6b02054

Xu, Z. Y.; Jiang, Y. Y.; Su, W.; Yu, H. Z.; Fu, Y.

Mechanism of Ligand-Controlled Regioselectivity-Switchable Copper-Catalyzed Alkylboration of Alkenes

Chemistry-a European Journal, (22): 14611-14617. 2016. 10.1002/chem.201602610

Xue, Y. S.; Wang, Y. H.; Cao, Z. Y.; Zhou, J.; Chen, Z. X.

Computational insight into the cooperative role of non-covalent interactions in the aza-Henry reaction catalyzed by quinine derivatives: mechanism and enantioselectivity

Organic & Biomolecular Chemistry, (14): 9588-9597. 2016. 10.1039/c6ob01611a

Yadav, M. P. S.; Kumar, A.; Jayarama, A.

Vibrational spectra analysis, NBO, HOMO-LUMO, and nonlinear optical behavior studies on 3-(3,4-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one

Monatshefte fur Chemie, (147): 1045-1061. 2016. 10.1007/s00706-015-1567-8

Yamada, M.; Tanabe, Y.; Dang, J. S.; Sato, S.; Mizorogi, N.; Hachiya, M.; Suzuki, M.; Abe, T.; Kurihara, H.; Maeda, Y.; Zhao, X.; Lian, Y. F.; Nagase, S.; Akasaka, T.

D-2d(23)-C-84 versus Sc₂C₂@D-2d(23)-C-84: Impact of Endohedral Sc₂C₂ Doping on Chemical Reactivity in the Photolysis of Diazirine

Journal of the American Chemical Society, (138): 16523-16532. 2016. 10.1021/jacs.6b10751

Yamamura, M.; Nabeshima, T.

Relationship between the Bowl-Shaped Geometry of Phosphangulene and an Axial Group on the Phosphorus Atom

Bulletin of the Chemical Society of Japan, (89): 42-49. 2016. 10.1246/bcsj.20150288

Yamashita, M.

The Organometallic Chemistry of Boron-Containing Pincer Ligands based on Diazaboroles and Carboranes
Bulletin of the Chemical Society of Japan, (89): 269-281. 2016. 10.1246/bcsj.20150355

Yan, X. L.; Li, X. Y.; Sun, Z.; Li, Q. Z.; Meng, L. P.

Dinuclear first-row transition metal-(C₈Me₆)₂ complexes: metal-metal and metal-ligand bonds determined by the d electron configuration of the metal atom
New Journal of Chemistry, (40): 1988-1996. 2016. 10.1039/c5nj02469b

Yan, X. L.; Meng, L. P.; Sun, Z.; Li, X. Y.

*Metal-metal bonding and aromaticity in M-2(NHCHNH)(3) (2) (*mu*-E)(2) (E=O, S; M=Nb, Mo, Tc, Ru, Rh)*
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2912-5

Yan, Z. E.; Huo, R. P.; Guo, L. H.; Zhang, X.

The mechanisms for N-heterocyclic olefin-catalyzed formation of cyclic carbonate from CO₂ and propargylic alcohols
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2959-3

Yandanova, E. S.; Ivanov, D. M.; Kuznetsov, M. L.; Starikov, A. G.; Starova, G. L.; Kukushkin, V. Y.

Recognition of S center dot center dot center dot Cl Chalcogen Bonding in Metal-Bound Alkylthiocyanates
Crystal Growth & Design, (16): 2979-2987. 2016. 10.1021/acs.cgd.6b00346

Yang, C.; Zhang, E. G.; Li, X.; Cheng, J. P.

Asymmetric Conjugate Addition of Benzofuran-2-ones to Alkyl 2-Phthalimidoacrylates: Modeling Structure-Stereoselectivity Relationships with Steric and Electronic Parameters
Angewandte Chemie-International Edition, (55): 6506-6510. 2016. 10.1002/anie.201601028

Yang, D. P.; Zheng, R.; Wang, Y. S.; Lv, J.

Theoretical investigation on ESIPT mechanism of a new fluorescent sensor in different solvents
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (159): 30-34. 2016. 10.1016/j.saa.2016.01.025

Yang, H. H.; Chen, H. S.

The stabilities and electronic structures of Al_nSi_{12-n}N₁₂ (n=0, 1, 2, and 4)
Journal of Materials Research, (31): 241-249. 2016. 10.1557/jmr.2015.390

Yang, H. Q.; Wang, X.; Ma, Y.; Wang, L.; Zhang, J. L.

Quaternary ammonium-based ionic liquids bearing different numbers of hydroxyl groups as highly efficient catalysts for the fixation of CO₂: a theoretical study by QM and MD
Catalysis Science & Technology, (6): 7773-7782. 2016. 10.1039/c6cy01045h

Yang, J.; Chen, J.; Li, Z. B.

Structural Basis for the Structure-Activity Behaviour of Oxaliplatin and its Enantiomeric Analogues: A Molecular Dynamics Study of Platinum-DNA Intrastrand Crosslink Adducts
Australian Journal of Chemistry, (69): 379-387. 2016. 10.1071/ch15624

Yang, N.; Liao, Q.; Li, Q.; Zhang, P.; Li, L. Q.

Simple and easy-operated method for filtering eco-friendly corrosion inhibitors
Anti-Corrosion Methods and Materials, (63): 73-81. 2016. 10.1108/acmm-07-2014-1406

Yang, X.; Yang, Y. S.; Rees, R. J.; Yang, Q.; Tian, Z. Y.; Xue, Y.

How Dirhodium Catalyst Controls the Enantioselectivity of 3+2 -Cycloaddition between Nitrone and Vinyldiazoacetate: A Density Functional Theory Study
Journal of Organic Chemistry, (81): 8082-8086. 2016. 10.1021/acs.joc.6b01447

Yang, X.; Yang, Y. S.; Xue, Y.

Computational Mechanism Study of Catalyst-Dependent Competitive 1,2-C → C, -O → C, and -N → C Migrations from beta-Methylene-beta-silyloxy-beta-amido-alpha-diazoacetate: Insight into the Origins of Chemoselectivity
ACS Catalysis, (6): 162-175. 2016. 10.1021/acscatal.5b02103

- Yang, Y. F.; Houk, K. N.; Wu, Y. D.
Computational Exploration of Rh-III/Rh-V and Rh-III/Rh-I Catalysis in Rhodium(III)-Catalyzed C-H Activation Reactions of N-Phenoxyacetamides with Alkynes
Journal of the American Chemical Society, (138): 6861-6868. 2016. 10.1021/jacs.6b03424
- Yankova, R.; Genieva, S.; Halachev, N.; Dimitrova, G.
Molecular structure, vibrational spectra, MEP, HOMO-LUMO and NBO analysis of Hf(SeO₃)(SeO₄)(H₂O)(4)
Journal of Molecular Structure, (1106): 82-88. 2016. 10.1016/j.molstruc.2015.10.091
- Yeh, Y. H.; Gorte, R. J.; Rangarajan, S.; Mavrikakis, M.
Adsorption of Small Alkanes on ZSM-5 Zeolites: Influence of Bronsted Sites
Journal of Physical Chemistry C, (120): 12132-12138. 2016. 10.1021/acs.jpcc.6b03855
- Yildiz, C. B.; Azizoglu, A.
Substituent effects on the ring-opening mechanism of gem-dibromospiropentanes to related allenes: a theoretical study
Journal of Physical Organic Chemistry, (29): 63-68. 2016. 10.1002/poc.3487
- Yin, S.; Bernstein, E. R.
Properties of iron sulfide, hydrosulfide, and mixed sulfide/hydrosulfide cluster anions through photoelectron spectroscopy and density functional theory calculations
Journal of Chemical Physics, (145) 2016. 10.1063/1.4964651
- Yin, Y. B.
DFT study on deprotonation and protonation of porphyrins: How many protons can the porphyrin core take up?
Computational and Theoretical Chemistry, (1080): 38-46. 2016. 10.1016/j.comptc.2016.01.022
- Yokogawa, D.
Time-dependent density functional theory (TD-DFT) coupled with reference interaction site model self-consistent field explicitly including spatial electron density distribution (RISM-SCF-SEDD)
Journal of Chemical Physics, (145) 2016. 10.1063/1.4962062
- Yoosefian, M.; Ansarinik, Z.; Etminan, N.
Density functional theory computational study on solvent effect, molecular conformations, energies and intramolecular hydrogen bond strength in different possible nano-conformers of acetaminophen
Journal of Molecular Liquids, (213): 115-121. 2016. 10.1016/j.molliq.2015.10.060
- Yoosefian, M.; Etminan, N.
Density functional theory (DFT) study of a new novel bionanosensor hybrid; tryptophan/Pd doped single walled carbon nanotube
Physica E-Low-Dimensional Systems & Nanostructures, (81): 116-121. 2016. 10.1016/j.physe.2016.03.009
- Yoosefian, M.; Etminan, N.
The role of solvent polarity in the electronic properties, stability and reactivity trend of a tryptophane/Pd doped SWCNT novel nanobiosensor from polar protic to non-polar solvents
RSC Advances, (6): 64818-64825. 2016. 10.1039/c6ra14006h
- Yoosefian, M.; Etminan, N.; Moghani, M. Z.; Mirzaei, S.; Abbasi, S.
The role of boron nitride nanotube as a new chemical sensor and potential reservoir for hydrogen halides environmental pollutants
Superlattices and Microstructures, (98): 325-331. 2016. 10.1016/j.spmi.2016.08.049
- York, J. T.
Determining the Impact of Ligand and Alkene Substituents on Bonding in Gold(I)-Alkene Complexes Supported by N-Heterocyclic Carbenes: A Computational Study
Journal of Physical Chemistry A, (120): 6064-6075. 2016. 10.1021/acs.jpca.6b03819

- You, X. R.; Tian, W. J.; Li, D. Z.; Wang, Y. J.; Li, R.; Feng, L. Y.; Zhai, H. J.
On the nature of chemical bonding in the all-metal aromatic Sb₃Au₃Sb₃ (3-) sandwich complex
Physical Chemistry Chemical Physics, (18): 13423-13431. 2016. 10.1039/c6cp00101g
- Yu, D.; Wu, D.; Li, Y.; Li, S. Y.
On the formation of beryllium bonds where radicals act as electron donors
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1877-x
- Yu, D. H.; Du, R. B.; Xiao, J. C.
pKa Prediction for Acidic Phosphorus-Containing Compounds Using Multiple Linear Regression with Computational Descriptors
Journal of Computational Chemistry, (37): 1668-1671. 2016. 10.1002/jcc.24381
- Yu, K.; Liu, X. Y.; Qi, T.; Yang, H. Q.; Whitfield, D. M.; Chen, Q. Y.; Huisman, E. J. C.; Hu, C. W.
General low-temperature reaction pathway from precursors to monomers before nucleation of compound semiconductor nanocrystals
Nature Communications, (7) 2016. 10.1038/ncomms12223
- Yu, X.; Zhu, H. R.; Zeng, Y.
A DFT study of Lp center dot center dot center dot/halogen bond competition in complexes of perhalogenated alkenes with oxygen/nitrogen containing simple molecules
International Journal of Quantum Chemistry, (116): 1244-1253. 2016. 10.1002/qua.25166
- Yu, X. H.; Oganov, A. R.; Popov, I. A.; Boldyrev, A. I.
d-AO Spherical Aromaticity in Ce₆O₈
Journal of Computational Chemistry, (37): 103-109. 2016. 10.1002/jcc.24049
- Yu, X. H.; Oganov, A. R.; Popov, I. A.; Qian, G. R.; Boldyrev, A. I.
Antiferromagnetic Stabilization in the Ti₈O₁₂ Cluster
Angewandte Chemie-International Edition, (55): 1699-1703. 2016. 10.1002/anie.201508439
- Yuan, B.; Shin, J. W.; Bernstein, E. R.
Dynamics and fragmentation of van der Waals and hydrogen bonded cluster cations: (NH₃)_(n) and (NH₃BH₃)_(n) ionized at 10.51 eV
Journal of Chemical Physics, (144) 2016. 10.1063/1.4945624
- Yuan, C. Q.; An, P.; Chen, J.; Luo, Z. X.; Yao, J. N.
Unraveling weak interactions in aniline-pyrrole dimer clusters
Science China-Chemistry, (59): 1270-1276. 2016. 10.1007/s11426-016-0105-8
- Yuan, C. Q.; Wu, H. M.; Jia, M. Y.; Su, P. F.; Luo, Z. X.; Yao, J. N.
A theoretical study of weak interactions in phenylenediamine homodimer clusters
Physical Chemistry Chemical Physics, (18): 29249-29257. 2016. 10.1039/c6cp04922b
- Yuan, C. X.; Zhao, X. F.; Wu, Y. B.; Wang, X. T.
Ultrashort Beryllium-Beryllium Distances Rivalling Those of Metal-Metal Quintuple Bonds Between Transition Metals
Angewandte Chemie-International Edition, (55): 15651-15655. 2016. 10.1002/anie.201609455
- Yuan, H. Y.; Zheng, Y. Y.; Zhang, J. P.
Understanding the Mechanism of the Lewis Acid Promoted 3+2 Cycloaddition of Propargylic Alcohol and alpha-Oxo Ketene Dithioacetals
Journal of Organic Chemistry, (81): 1989-1997. 2016. 10.1021/acs.joc.5b02826
- Yuan, J.; Long, X. P.; Zhang, C. Y.
Influence of N-Oxide Introduction on the Stability of Nitrogen-Rich Heteroaromatic Rings: A Quantum Chemical Study
Journal of Physical Chemistry A, (120): 9446-9457. 2016. 10.1021/acs.jpca.6b08852
- Yuan, J. Y.; Li, G. W.; Yang, B. C.; Zhang, J. P.; Li, Z. J.; Chen, H. Y.

Selective adsorption of ethylene on bimetallic CuV_n (+/0) (n=1-5) clusters: A theoretical study
Computational Materials Science, (111): 489-496. 2016. 10.1016/j.commatsci.2015.09.064

Yuan, J. Y.; Wang, P.; Hou, G. L.; Peng, G.; Zhang, W. J.; Xu, X. L.; Xu, H. G.; Yang, J. L.; Zheng, W. J.
Structural Evolution and Electronic Properties of VnC₂₀/- and VnC₄₀/- (n=1-6) Clusters: Insights from Photoelectron Spectroscopy and Theoretical Calculations
Journal of Physical Chemistry A, (120): 1520-1528. 2016. 10.1021/acs.jpca.6b00241

Yuan, J. Y.; Yuan, Y. Z.; Tian, X. H.; Sun, J. Y.; Ge, Y.
Spirooxazine-Fulgide Biphotochromic Molecular Switches with Nonlinear Optical Responses across Four States
Journal of Physical Chemistry C, (120): 14840-14853. 2016. 10.1021/acs.jpcc.6b04849

Yuan, L.; Yu, H. T.
A Density Functional Theory Investigation of the Tandem Radical Cyclization of 1- 2-YI-3-(2-Methoxyphenyl)-prop2-enyl-6-oxo-1,6-dihdropyridine-2-carb onitrile
Australian Journal of Chemistry, (69): 319-327. 2016. 10.1071/ch15369

Yuan, P.; Zhang, T. T.; Cai, A. F.; Cui, C. S.; Liu, H. Y.; Bao, X. J.
Theoretical study on the mechanism of oxidative-extractive desulfurization in imidazolium-based ionic liquid
RSC Advances, (6): 74929-74936. 2016. 10.1039/c6ra16731d

Yuan, R. M.; Hu, R.; Fu, G.
Mechanistic Insight into the Copper-Catalyzed Regiodivergent Silacarboxylation of Allenes with CO₂
Chemistry-an Asian Journal, (11): 2201-2209. 2016. 10.1002/asia.201600739

Yuan, X. G.; Wang, W. M.; Tian, Z. Q.; Bi, S. W.; Ma, J.
Electron-donating groups and high ring strain promoted ring opening of methylenecyclopropanes catalyzed by rhodium and iridium complexes
Journal of Organometallic Chemistry, (811): 29-39. 2016. 10.1016/j.jorgchem.2016.03.006

Yuan, X. G.; Zheng, D.; Wang, X. Z.; Liu, P. Y.; Ma, J.
Unconventional O-H center dot center dot center dot C Hydrogen Bonding and Effects of Conformational Changes on Infrared Spectroscopy of o-Cresol in Solutions
Journal of Physical Chemistry A, (120): 10196-10206. 2016. 10.1021/acs.jpca.6b06945

Yuan, Y. L.; Chen, P. Y.; Yang, L. H.; Ju, Y.; Wang, H. M.
Quantum chemical insight into the reactivity of 1,3-dipoles on coronene as model for nanographenes
Russian Journal of Physical Chemistry A, (90): 173-182. 2016. 10.1134/s0036024416010337

Yuce, A. O.; Telli, E.; Mert, B. D.; Kardas, G.; Yazici, B.
Experimental and quantum chemical studies on corrosion inhibition effect of 5,5 diphenyl 2-thiohydantoin on mild steel in HCl solution
Journal of Molecular Liquids, (218): 384-392. 2016. 10.1016/j.molliq.2016.02.087

Yuvaraj, K.; Bhattacharyya, M.; Prakash, R.; Ramkumar, V.; Ghosh, S.
New Trinuclear Complexes of Group 6, 8, and 9 Metals with a Triply Bridging Borylene Ligand
Chemistry-a European Journal, (22): 8889-8896. 2016. 10.1002/chem.201600637

Zaater, S.; Bouchoucha, A.; Djebbar, S.; Brahimi, M.
Structure, vibrational analysis, electronic properties and chemical reactivity of two benzoxazole derivatives: Functional density theory study
Journal of Molecular Structure, (1123): 344-354. 2016. 10.1016/j.molstruc.2016.06.047

Zabardasti, A.; Sharifi-Rad, A.
A new approach on diminutive effects for non-covalent interactions: fused bicyclic hydrogen-bonded complexes of hypohalous acids with fluoromethanol
Molecular Physics, (114): 3341-3355. 2016. 10.1080/00268976.2016.1232445

- Zabardasti, A.; Talebi, N.; Kakanejadifard, A.; Saki, Z.
The B-C and C-C bonds as preferred electron source for H-bond and Li-bond interactions in complex pairing of C4B2H6 with HF and LiH molecules
Structural Chemistry, (27): 573-581. 2016. 10.1007/s11224-015-0586-8
- Zabojnikova, T.; Cajzl, R.; Kljun, J.; Chval, Z.; Turel, I.; Burda, J. V.
Interactions of the "piano-stool" ruthenium(II)((6)-arene)(quinolone)Cl (+) complexes with water; DFT computational study
Journal of Computational Chemistry, (37): 1766-1780. 2016. 10.1002/jcc.24373
- Zahedi, E.; Babaie, M.; Bahmanpour, H.
Adsorption properties of boroxol ring doped zigzag boron nitride nanotube toward NO molecule using DFT
International Journal of Modern Physics B, (30) 2016. 10.1142/s0217979216501010
- Zahedi, E.; Yari, M.; Bahmanpour, H.
Adsorption of carbon monoxide on boroxol-ring-doped zigzag boron nitride nanotube: Electronic study via DFT
European Physical Journal Plus, (131) 2016. 10.1140/epjp/i2016-16120-9
- Zakarianezhad, M.; Masoodi, H. R.; Shool, M.
Theoretical study of the mechanism of stable phosphorus ylides derived from 2-aminothiophenol in the presence of different dialkyl acetylenedicarboxylates
Phosphorus Sulfur and Silicon and the Related Elements, (191): 1063-1068. 2016. 10.1080/10426507.2016.1138305
- Zamani, M.
Density functional study of the structure and water adsorption activity of an Al₂O₃ star-shaped alumina nanocage
Turkish Journal of Chemistry, (40): 54-64. 2016. 10.3906/kim-1501-69
- Zamani, M.
Surface study and sensing activity of nanotubular indium trioxide to NH₃, H₂S, NO₂ and CO environmental pollutants
Applied Surface Science, (363): 421-431. 2016. 10.1016/j.apsusc.2015.12.014
- Zanatta, G.; Nunes, G. D.; Bezerra, E. M.; da Costa, R. F.; Martins, A.; Caetano, E. W. S.; Freire, V. N.; Gottfried, C.
Two Binding Geometries for Risperidone in Dopamine D3 Receptors: Insights on the Fast-Off Mechanism through Docking, Quantum Biochemistry, and Molecular Dynamics Simulations
ACS Chemical Neuroscience, (7): 1331-1347. 2016. 10.1021/acschemneuro.6b00074
- Zapata-Escobar, A. D.; Carcamo-Camacho, T.; Hadad, C. Z.; Restrepo, A.
On the nature of the trimer, tetramer, and pentamer of ammonia borane
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1853-5
- Zeng, G. X.; Maeda, S.; Taketsugu, T.; Sakaki, S.
Theoretical Study of Hydrogenation Catalysis of Phosphorus Compound and Prediction of Catalyst with High Activity and Wide Application Scope
ACS Catalysis, (6): 4859-4870. 2016. 10.1021/acscatal.5b02968
- Zeng, Q.; Li, J. S.; Huang, H.; Wang, X. Q.; Yang, M. L.
Polarization response of clathrate hydrates capsulated with guest molecules
Journal of Chemical Physics, (144) 2016. 10.1063/1.4952417
- Zeng, Q.; Li, Z. C.; Wang, Y. B.; Zhai, H. Q.; Tao, O.; Wang, Y.; Guan, J.; Zhang, Y. Y.
Substituent effects on gas-phase homolytic Fe-O and Fe-S bond energies of m-G-C₆H₄OFe(CO)(2)(eta(5)-C₅H₅) and m-G-C₆H₄SFe(CO)(2)(eta(5)-C₅H₅) studied using Hartree-Fock and density functional theory methods
Journal of Physical Organic Chemistry, (29): 172-184. 2016. 10.1002/poc.3514
- Zhang, C. G.; Lv, X. Y.; Lu, G.; Wang, Z. X.
Metal-free homolytic hydrogen activation: a quest through density functional theory computations
New Journal of Chemistry, (40): 8141-8148. 2016. 10.1039/c6nj00557h

- Zhang, F. T.; Cui, G. K.; Zhao, N.; Huang, Y. J.; Zhao, Y. L.; Wang, J. J.
Improving SO₂ capture by basic ionic liquids in an acid gas mixture (10% vol SO₂) through tethering a formyl group to the anions
RSC Advances, (6): 86082-86088. 2016. 10.1039/c6ra18589d
- Zhang, F. Y.; Sui, H. G.; Zhao, L. M.; Guo, Y. H.; Tang, L.; Guo, W. Y.
Theoretical investigation of the reaction of ethanol with ground-state Co+(F-3)
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-2000-z
- Zhang, F. Y.; Yu, P.; Xu, Y. Y.; Shen, W.; Li, M.; He, R. X.
Theoretical investigation of regeneration mechanism of the metal-free sensitizer in dye sensitized solar cells
Dyes and Pigments, (124): 156-164. 2016. 10.1016/j.dyepig.2015.08.023
- Zhang, G. Q.; Li, H.; Weinhold, F.; Chen, D. Z.
3c/4e (sigma)over-cap-type long-bonding competes with omega-bonding in noble-gas hydrides HNgY (Ng = He, Ne, Ar, Kr, Xe, Rn; Y = F, Cl, Br, I): a NBO/NRT perspective
Physical Chemistry Chemical Physics, (18): 8015-8026. 2016. 10.1039/c5cp07965a
- Zhang, G. X.; Qi, Y. H.; Xu, C. J.
Theoretical study on the substitution reactions of the germyleenoid H₂GeLiF with SiH₃X (X = F, Cl, Br)
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2997-x
- Zhang, H.; Zhang, H. M.; Wang, L. J.; Shen, J. Y.
Density Functional Theory Studies on the CO₂ Absorption by 1-Ethylamine-3-methylimidazolium Tetrafluoroborate
Chemical Journal of Chinese Universities-Chinese, (37): 1660-1668. 2016. 10.7503/cjcu20160337
- Zhang, H. Y.; Jiang, X. Y.; Wu, W.; Mo, Y. R.
Electron conjugation versus pi-pi repulsion in substituted benzenes: why the carbon-nitrogen bond in nitrobenzene is longer than in aniline
Physical Chemistry Chemical Physics, (18): 11821-11828. 2016. 10.1039/c6cp00471g
- Zhang, H. Y.; Wu, W.; Ahmed, B. M.; Mezei, G.; Mo, Y. R.
Adjacent Lone Pair (ALP) Effect: A Computational Approach for Its Origin
Chemistry-a European Journal, (22): 7415-7421. 2016. 10.1002/chem.201600509
- Zhang, J.; Dai, G. L.; Wu, F. S.; Li, D.; Gao, D. C.; Jin, H. W.; Chen, S.; Zhu, X. J.; Huang, C. X.; Han, D. M.
Efficient and tunable phosphorescence of new platinum(II) complexes based on the donor-pi-acceptor Schiff bases
Journal of Photochemistry and Photobiology a-Chemistry, (316): 12-18. 2016. 10.1016/j.jphotochem.2015.09.018
- Zhang, J.; Xie, J.; Lee, M. E.; Zhang, L.; Zuo, Y. J.; Feng, S. Y.
Ionic S(N)i-Si Nucleophilic Substitution in N-Methylaniline-Induced Si-Si Bond Cleavages of Si₂Cl₆
Chemistry-a European Journal, (22): 5010-5016. 2016. 10.1002/chem.201504927
- Zhang, J. H.; Kong, Q. H.; Yang, L. W.; Wang, D. Y.
Few layered Co(OH)(2) ultrathin nanosheet-based polyurethane nanocomposites with reduced fire hazard: from eco-friendly flame retardance to sustainable recycling
Green Chemistry, (18): 3066-3074. 2016. 10.1039/c5gc03048j
- Zhang, L.; Fang, D. C.
An Explicit Interpretation of the Directing Group Effect for the Pd(OAc)₂-Catalyzed Aromatic C-H Activations
Journal of Organic Chemistry, (81): 7400-7410. 2016. 10.1021/acs.joc.6b00997
- Zhang, L.; Ju, M. G.; Liang, W. Z.
The effect of moisture on the structures and properties of lead halide perovskites: a first-principles theoretical investigation
Physical Chemistry Chemical Physics, (18): 23174-23183. 2016. 10.1039/c6cp01994c
- Zhang, L.; Li, W.; Fang, T.; Li, S. H.

Ab initio molecular dynamics with intramolecular noncovalent interactions for unsolvated polypeptides
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-015-1799-z

Zhang, L.; Zhang, C. Y.; Song, X. H.; Wang, B. Q.; Zhang, J.
Geometries, stabilities, electronic and magnetic properties of small aluminum cluster anions doped with cobalt: A density functional theory study
Journal of Structural Chemistry, (57): 33-46. 2016. 10.1134/s0022476616010054

Zhang, L. H.; Yu, M. D.; Peng, Q.; Zhao, H. B.; Gao, J. W.
Molecular design and theoretical investigation on the thieno 3,2-b thienobis(silolothiophene)-based low band gap donor polymers for efficient polymer solar cell
Molecular Simulation, (42): 47-55. 2016. 10.1080/08927022.2015.1008469

Zhang, L. J.; Liu, S.; Cheng, M.; Du, Y. K.; Zhu, Q. H.
Vibrational Spectra and Theoretical Calculations of cis- and trans-3Fluoro-N-methylaniline in the Neutral (S-0) and Cationic (D-0) Ground States
Journal of Physical Chemistry A, (120): 81-94. 2016. 10.1021/acs.jpca.5b11991

Zhang, L. J.; Su, J.; Yang, S. T.; Guo, X. J.; Jia, Y. P.; Chen, N.; Zhou, J.; Zhang, S.; Wang, S.; Li, J.; Li, J. Y.; Wu, G. Z.; Wang, J. Q.
Extended X-ray Absorption Fine Structure and Density Functional Theory Studies on the Complexation Mechanism of Amidoximate Ligand to Uranyl Carbonate
Industrial & Engineering Chemistry Research, (55): 4224-4230. 2016. 10.1021/acs.iecr.5b03217

Zhang, L. S.; Li, H. F.; Li, X.; Fan, X. L.
Ligand modification effects on the electrochromic character of ruthenium sulfoxide complexes: a theoretical perspective
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1947-0

Zhang, N.; Geronimo, I.; Paneth, P.; Schindelka, J.; Schaefer, T.; Herrmann, H.; Vogt, C.; Richnow, H. H.
Analyzing sites of OH radical attack (ring vs. side chain) in oxidation of substituted benzenes via dual stable isotope analysis (delta C-13 and delta H-2)
Science of the Total Environment, (542): 484-494. 2016. 10.1016/j.scitotenv.2015.10.075

Zhang, Q.; Du, L.
Hydrogen bonding in the carboxylic acid-aldehyde complexes
Computational and Theoretical Chemistry, (1078): 123-128. 2016. 10.1016/j.comptc.2016.01.007

Zhang, Q. N.; Qu, H.; Chen, M. H.; Zhou, M. F.
Carbon Dioxide Activation by Scandium Atoms and Scandium Monoxide Molecules: Formation and Spectroscopic Characterization of ScCO₃ and OCScCO₃ in Solid Neon
Journal of Physical Chemistry A, (120): 425-432. 2016. 10.1021/acs.jpca.5b11809

Zhang, S. Y.; Chen, J. W.; Zhao, Q.; Xie, Q.; Wei, X. X.
Unveiling self-sensitized photodegradation pathways by DPT calculations: A case of sunscreen p-aminobenzoic acid
Chemosphere, (163): 227-233. 2016. 10.1016/j.chemosphere.2016.08.028

Zhang, S. Z.; Wang, G. M.; Lu, Y. X.; Zhu, W. L.; Peng, C. J.; Liu, H. L.
The Interactions between Imidazolium-Based Ionic Liquids and Stable Nitroxide Radical Species: A Theoretical Study
Journal of Physical Chemistry A, (120): 6089-6102. 2016. 10.1021/acs.jpca.6b05770

Zhang, W.; Wang, Y.; Wei, D. H.; Tang, M. S.; Zhu, X. J.
A DFT study on NHC-catalyzed intramolecular aldehyde-ketone crossed-benzoin reaction: mechanism, regioselectivity, stereoselectivity, and role of NHC
Organic & Biomolecular Chemistry, (14): 6577-6590. 2016. 10.1039/c6ob00791k

Zhang, X. F.; Cao, Z. X.
Insight into the reaction mechanisms for oxidative addition of strong sigma bonds to an Al(I) center
Dalton Transactions, (45): 10355-10365. 2016. 10.1039/c6dt01154c

- Zhang, X. F.; Sun, M. J.; Cao, Z. X.
Theoretical study on interactions of N-heterocyclic carbene with the bare first-row transition metals
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1922-9
- Zhang, X. H.; Geng, Z. Y.
Mechanism of the gold(I)-catalyzed synthesis of imidazo-pyrimidines and imidazo-pyrazines via 3+2 dipolar cycloaddition: a DFT study
RSC Advances, (6): 62099-62108. 2016. 10.1039/c6ra07780c
- Zhang, X. N.; McRose, D. L.; Darnajoux, R.; Bellenger, J. P.; Morel, F. M. M.; Kraepiel, A. M. L.
Alternative nitrogenase activity in the environment and nitrogen cycle implications
Biogeochemistry, (127): 189-198. 2016. 10.1007/s10533-016-0188-6
- Zhang, X. P.; Liu, X. P.; Phillips, D. L.; Zhao, C. Y.
Mechanistic Insights Into the Factors That Influence the DNA Nuclease Activity of Mononuclear Facial Copper Complexes Containing Hetero-Substituted Cyclens
ACS Catalysis, (6): 248-257. 2016. 10.1021/acscatal.5b01735
- Zhang, X. P.; Xu, H. Y.; Liu, X. P.; Phillips, D. L.; Zhao, C. Y.
Mechanistic Insight into the Intramolecular Benzylic C-H Nitrene Insertion Catalyzed by Bimetallic Paddlewheel Complexes: Influence of the Metal Centers
Chemistry-a European Journal, (22): 7288-7297. 2016. 10.1002/chem.201600371
- Zhang, Y.; Zhang, Y.; Qi, Z. H.; Gao, Y.; Liu, W.; Wang, Y.
Ammonia-borane dehydrogenation catalyzed by Iron pincer complexes: A concerted metal-ligand cooperation mechanism
International Journal of Hydrogen Energy, (41): 17208-17215. 2016. 10.1016/j.ijhydene.2016.07.209
- Zhang, Z. F.; Ma, N. N.; Xuan, X. P.
An unusual C=C center dot center dot center dot C=O interaction in (Z)-3-(4-halogenphenyl)amino -2-cyanoprop-2-enoates
New Journal of Chemistry, (40): 85-88. 2016. 10.1039/c5nj01814e
- Zhao, C. X.; Lu, Y. X.; Wang, G. M.; Zhu, W. L.
Cation-anion radical interactions between halopyridinium cations and metal dithiolene complexes M(C₂S₂)₂CN (-center dot): A theoretical study of halogen bonds in conducting or magnetic molecular materials
International Journal of Quantum Chemistry, (116): 1872-1881. 2016. 10.1002/qua.25293
- Zhao, H. L.; Tang, S. S.; Li, S. Y.; Ding, L.; Du, L.
Theoretical investigation of the hydrogen bond interactions of methanol and dimethylamine with hydrazone and its derivatives
Structural Chemistry, (27): 1241-1253. 2016. 10.1007/s11224-016-0749-2
- Zhao, H. M.; Zhou, J.; Jena, P.
Stability of B-12(CN)₁₂(2-): Implications for Lithium and Magnesium Ion Batteries
Angewandte Chemie-International Edition, (55): 3704-3708. 2016. 10.1002/anie.201600275
- Zhao, J.; Du, J.; Liu, S.; Yang, Z. Z.; Zhao, D. X.; Liu, C.
Theoretical Studies on the Effect of Amino Acid Side Chains on Hydrogen Bonding for G : C in Aqueous Solution
Chemical Journal of Chinese Universities-Chinese, (37): 1686-1693. 2016. 10.7503/cjcu20160270
- Zhao, J.; Xu, B.; Yu, W. J.; Wang, X. F.
Silicon Tetrahydroborate and Silylene Dihydroborate with Interelement B-H-Si and B=Si Bonds
Organometallics, (35): 3272-3280. 2016. 10.1021/acs.organomet.6b00368
- Zhao, J. F.; Yang, Y.

Excited state proton transfer coupled with twisted intermolecular charge transfer for N,N-dimethylanilino-1,3-diketone in high polar acetonitrile solvent
Journal of Molecular Liquids, (220): 735-741. 2016. 10.1016/j.molliq.2016.05.029

Zhao, J. X.; Gao, Q.; Zhang, F. F.; Sun, W.; Bai, Y. J.
Two colorimetric fluorescent probes for detection Fe³⁺: Synthesis, characterization and theoretical calculations
Journal of Luminescence, (180): 278-286. 2016. 10.1016/j.jlumin.2016.07.037

Zhao, L. J.; Tian, W. J.; Ou, T.; Xu, H. G.; Feng, G.; Xu, X. L.; Zhai, H. J.; Li, S. D.; Zheng, W. J.
Structures and chemical bonding of B₃O₃-/0 and B₃O₃H-/0: A combined photoelectron spectroscopy and first-principles theory study
Journal of Chemical Physics, (144) 2016. 10.1063/1.4943768

Zhao, L. J.; Xu, H. G.; Feng, G.; Wang, P.; Xu, X. L.; Zheng, W. J.
Superhalogen properties of BS₂- and BSO₂-: photoelectron spectroscopy and theoretical calculations
Physical Chemistry Chemical Physics, (18): 6175-6181. 2016. 10.1039/c5cp07673k

Zhao, Q.
Cooperative effects between halogen bonds and pnictogen bonds in XBr center dot center dot center dot OFH₂P center dot center dot center dot NH₃ (X = F, Cl, CN, NC, OH, and NO₂) complexes
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-015-2872-1

Zhao, Q.; Ng, S. S. H.; Kulik, H. J.
Predicting the Stability of Fullerene Allotropes Throughout the Periodic Table
Journal of Physical Chemistry C, (120): 17035-17045. 2016. 10.1021/acs.jpcc.6b04361

Zhao, R. S.; Guo, Y. J.; Zhao, P.; Ehara, M.; Nagase, S.; Zhao, X.
Warning to Theoretical Structure Elucidation of Endohedral Metallofullerenes
Journal of Physical Chemistry C, (120): 1275-1283. 2016. 10.1021/acs.jpcc.5b09403

Zhao, S. Z.; Teijaro, C. N.; Chen, H.; Sirasani, G.; Vaddypally, S.; Zdilla, M. J.; Dobereiner, G. E.; Andrade, R. B.
Concise Syntheses of bis-Strychnos Alkaloids (-)-Sungucine, (-)-Isosungucine, and (-)-Strychnogucine B from (-)-Strychnine
Chemistry-a European Journal, (22): 11593-11596. 2016. 10.1002/chem.201602663

Zhao, X. F.; Li, H. X.; Yuan, C. X.; Li, Y. Q.; Wu, Y. B.; Wang, Z. X.
Linear, Planar, and Tubular Molecular Structures Constructed by Double Planar Tetracoordinate Carbon D-2h C-2(BeH)(4) Species via Hydrogen-Bridged -BeH2Be- Bonds
Journal of Computational Chemistry, (37): 261-269. 2016. 10.1002/jcc.24018

Zhao, X. F.; Yuan, C. X.; Wang, X.; Li, J. J.; Wu, Y. B.; Wang, X. T.
Computational Design of Organometallic Oligomers Featuring 1,3-Metal-Carbon Bonding and Planar Tetracoordinate Carbon Atoms
Journal of Computational Chemistry, (37): 296-303. 2016. 10.1002/jcc.24185

Zhao, Y.; Yang, F.; Wang, J. R.; Yu, P. Y.; Pan, H. F.; Wang, H. F.; Wang, J. P.
Structural dynamics of nitrosylruthenium isomeric complexes studied with steady-state and transient pump-probe infrared spectroscopies
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (166): 62-67. 2016. 10.1016/j.saa.2016.04.055

Zhao, Y. L.; Yu, H. T.; Lian, Y. F.
Experimental and theoretical evaluation of structures of Pr-2@C-72 and its functionalized adduct with adamantylidene carbene
RSC Advances, (6): 115113-115119. 2016. 10.1039/c6ra23224h

Zhao, Y. L.; Zhou, Q.; Lian, Y. F.; Yu, H. T.
Experimental and theoretical investigation of structures and relative reactivity of Pr@C-74 and Pr@C-74(C₆H₃Cl₂)
Diamond and Related Materials, (64): 110-118. 2016. 10.1016/j.diamond.2016.02.004

- Zheng, D. Q.; Mao, R. Y.; Li, Z. M.; Wu, J.
A copper(I)-catalyzed three-component reaction of triethoxysilanes, sulfur dioxide, and alkyl halides
Organic Chemistry Frontiers, (3): 359-363. 2016. 10.1039/c5qo00399g
- Zheng, M.; Li, X. H.; Cui, H. L.; Zhang, R. Z.
Comparative Theoretical Studies on Several Energetic Substituted Dioxin-imidazole Derivatives
Chinese Journal of Chemical Physics, (29): 349-357. 2016. 10.1063/1674-0068/29/cjcp1506118
- Zheng, W. R.; Ding, L. L.; Wang, J. Y.; Wang, Y. X.
Computational study on alkenyl/aryl C(sp²)-O homolytic cleavage of carboxylates and carbamates
RSC Advances, (6): 26514-26525. 2016. 10.1039/c5ra27859g
- Zheng, Y. Z.; Zhou, Y.; Liang, Q.; Chen, D. F.; Guo, R.
Theoretical studies on the hydrogen-bonding interactions between luteolin and water: a DFT approach
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-3128-4
- Zheng, Y. Z.; Zhou, Y.; Liang, Q.; Chen, D. F.; Guo, R.
A theoretical study on the hydrogen-bonding interactions between flavonoids and ethanol/water
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2968-2
- Zheng, Y. Z.; Zhou, Y.; Liang, Q.; Chen, D. F.; Guo, R.; Lai, R. C.
Hydrogen-bonding Interactions between Apigenin and Ethanol/Water: A Theoretical Study
Scientific Reports, (6) 2016. 10.1038/srep34647
- Zhou, D. G.; Zhou, P. P.; Jing, H. W.
Mechanisms of cascade reactions between N-methylindole and sulfonylazides via Huisgen cycloaddition: A theoretical investigation
Journal of Molecular Catalysis a-Chemical, (417): 19-27. 2016. 10.1016/j.molcata.2016.03.010
- Zhou, F. F.; Liu, R. R.; Tang, J.; Li, P.; Cui, Y. H.; Zhang, H. Y.
On the properties of Se center dot center dot center dot N interaction: the analysis of substituent effects by energy decomposition and orbital interaction
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-015-2901-0
- Zhou, J. W.; Outlaw, V. K.; Townsend, C. A.; Bragg, A. E.
Quenching of pH-Responsive Luminescence of a Benzoindolizine Sensor by an Ultrafast Hydrogen Shift
Chemistry-a European Journal, (22): 15212-15215. 2016. 10.1002/chem.201603284
- Zhou, P. P.; Yang, X.; Ye, W. C.; Zhang, L. W.; Yang, F.; Zhou, D. G.; Liu, S. B.
Competition and cooperativity of sigma-hole and pi-hole intermolecular interactions between carbon monoxide and bromopentafluorobenzene
New Journal of Chemistry, (40): 9139-9147. 2016. 10.1039/c6nj01904h
- Zhou, S. D.; Li, J. L.; Schlangen, M.; Schwarz, H.
Mechanistic Aspects of the Holmium-Mediated, Reciprocal Hydrogen/Sulfur Exchange in the Gas Phase: C6H5CH3+CH2SC6H5CHS+CH4
Chemistry-a European Journal, (22): 4336-+. 2016. 10.1002/chem.201600061
- Zhou, T. W.; Wang, G. Q.; Cui, H.; Yuan, H. K.; Kuang, A. L.; Tian, C. L.; Wang, J. Z.; Chen, H.
A novel dehydrogenation style of NH3BH3 by catalyst of transition metal clusters
International Journal of Hydrogen Energy, (41): 11746-11760. 2016. 10.1016/j.ijhydene.2015.12.201
- Zhou, X. M.; Cao, B. B.; Liu, S. Y.; Sun, X. J.; Zhu, X.; Fu, H.
Theoretical and experimental investigation on the capture of H2S in a series of ionic liquids
Journal of Molecular Graphics & Modelling, (68): 87-94. 2016. 10.1016/j.jmgm.2016.06.013
- Zhou, X. M.; Cao, B. B.; Liu, S. Y.; Sun, X. J.; Zhu, X.; Fu, H.

Thermal reaction of the ionic liquid 1,2-dimethyl-(3-aminoethyl) imidazolium tetrafluoroborate: a kinetic and theoretical study
Journal of Molecular Modeling, (22) 2016. 10.1007/s00894-016-2996-y

Zhou, Y.; Deng, G.; Zheng, Y. Z.; Xu, J.; Ashraf, H.; Yu, Z. W.
Evidences for Cooperative Resonance-Assisted Hydrogen Bonds in Protein Secondary Structure Analogs
Scientific Reports, (6) 2016. 10.1038/srep36932

Zhou, Y. Q.; Fang, C. H.; Fang, Y.; Zhu, F. Y.; Liu, H. Y.; Ge, H. W.
Hydrogen generation mechanism of BH₄- spontaneous hydrolysis: A sight from ab initio calculation
International Journal of Hydrogen Energy, (41): 22668-22676. 2016. 10.1016/j.ijhydene.2016.10.057

Zhu, C.; Yang, G.
Insights from the Adsorption of Halide Ions on Graphene Materials
Chemphyschem, (17): 2482-2488. 2016. 10.1002/cphc.201600271

Zhu, C. Q.; Yang, C. X.; Wang, Y. H.; Lin, G.; Yang, Y. H.; Wang, X. Y.; Zhu, J.; Chen, X. Y.; Lu, X.; Liu, G.; Xia, H. P.
CCCCC pentadentate chelates with planar Möbius aromaticity and unique properties
Science Advances, (2) 2016. 10.1126/sciadv.1601031

Zhu, X. Y.; Ai, H. Q.
The Hygroscopy of Amino Acid Ionic Liquids in Aqueous Solution: a Quantum Chemistry Study
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics, (230): 1629-1640. 2016. 10.1515/zpch-2015-0685

Zicovich-Wilson, C. M.; Ho, M.; Navarrete-Lopez, A. M.; Casassa, S.
Hirshfeld-I charges in linear combination of atomic orbitals periodic calculations
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1942-5

Zierkiewicz, W.; Fanfrlik, J.; Hobza, P.; Michalska, D.; Zeegers-Huyskens, T.
Ab initio and DFT studies of the interaction between carbonyl and thiocarbonyl groups: the role of S center dot center dot O chalcogen bonds
Theoretical Chemistry Accounts, (135) 2016. 10.1007/s00214-016-1972-z

Zimmermann, L. W.; Van, N. D.; Gudat, D.; Schleid, T.
Bismuth Undecahydro-closo-dodecaborane: A Retainable Intermediate of B-H Bond Activation by Bismuth(III) Cations
Angewandte Chemie-International Edition, (55): 1909-1911. 2016. 10.1002/anie.201509629

Zolfigol, M. A.; Khazaei, A.; Alaie, S.; Baghery, S.; Maleki, F.; Bayat, Y.; Asgari, A.
Experimental and theoretical approving of anomeric based oxidation in the preparation of 2-sbstituted benz-(imida, oxa and othia)-zoles using 2,6-DMPy-NO₂ C(NO₂)(3) as a novel nano molten salt catalyst
RSC Advances, (6): 58667-58679. 2016. 10.1039/c6ra13231f

Zolghadr, A. R.; Dokooohaki, M. H.
Self-assembly of neuroprotective carbazolium based small molecules at octane/water interface: A simulation investigation
Chemical Physics, (480): 1-11. 2016. 10.1016/j.chemphys.2016.10.008

Zolghadr, A. R.; Ghatee, M. H.; Moosavi, F.
The effect of various quantum mechanically derived partial atomic charges on the bulk properties of chloride-based ionic liquids
Chemical Physics, (475): 23-31. 2016. 10.1016/j.chemphys.2016.05.022

Zou, W. L.; Cremer, D.
C-2 in a Box: Determining Its Intrinsic Bond Strength for the X-1 sigma(+)(g) Ground State
Chemistry-a European Journal, (22): 4087-4099. 2016. 10.1002/chem.201503750