

NBO 2010 (Jan-Dec) - 1009 references  
Compiled by Ariel Neff; Updated 4/16/13

Accorsi, G.; Armaroli, N.; Delavaux-Nicot, B.; Kaeser, A.; Holler, M.; Nierengarten, J.-F.; Esposti, A. D.  
*The electronic properties of a homoleptic bisphosphine Cu(I) complex A joint theoretical and experimental insight*  
Journal of Molecular Structure-Theochem, (962): 7-14 2010.

Acharjee, N.; Banerji, A.; Prange, T.  
*DFT study of 1,3-dipolar cycloadditions of C,N-disubstituted aldonitrones to chalcones evidenced by NMR and X-ray analysis*  
Monatshefte fur Chemie, (141): 1213-1221 2010.

Acosta-Silva, C.; Branchadell, V.; Bertran, J.; Oliva, A.  
*Mutual Relationship between Stacking and Hydrogen Bonding in DNA. Theoretical Study of Guanine-Cytosine, Guanine-5-methylcytosine, and Their Dimers*  
Journal of Physical Chemistry B, (114): 10217-10227 2010.

Adugna, S.; Revunova, K.; Djukic, B.; Gorelsky, S. I.; Jenkins, H. A.; Lemaire, M. T.  
*Persistent Metal Bis(Hexafluoroacetylacetonato) Complexes Featuring a 2,2'-Bipyridine Substituted Triarylamminium Radical Cation*  
Inorganic Chemistry, (49): 10183-10190 2010.

Afonin, A. V.  
*Through space spin-spin coupling F-19-H-1 as the base for comparative analysis of conformational equilibrium in fluorine-substituted aryl vinyl selenides and sulfides*  
Russian Journal of Organic Chemistry, (46): 1313-1316 2010.

Afonin, A. V.; Ushakov, I. A.; Pavlov, D. V.; Ivanov, A. V.; Mikhaleva, A. b. I.  
*Study of conformations and hydrogen bonds in the configurational isomers of pyrrole-2-carbaldehyde oxime by H-1, C-13 and N-15 NMR spectroscopy combined with MP2 and DFT calculations and NBO analysis*  
Magnetic Resonance in Chemistry, (48): 685-692 2010.

Afonin, A. V.; Ushakov, I. A.; Vashchenko, A. V.; Kondrashov, E. V.; Rulev, A. Y.  
*GIAO, DFT, AIM and NBO analysis of the N-H center dot center dot center dot O intramolecular hydrogen-bond influence on the (1)J(N,H) coupling constant in push-pull diaminoenones*  
Magnetic Resonance in Chemistry, (48): 661-670 2010.

Afonin, A. V.; Vashchenko, A. V.  
*Theoretical study of bifurcated hydrogen bonding effects on the (1)J(N,H), (1h)J(N,H), (2h)J(N,N) couplings and H-1, N-15 shieldings in model pyrroles*  
Magnetic Resonance in Chemistry, (48): 309-317 2010.

Aghabozorg, H.; Manteghi, F.; Ghadermazi, M.; Mirzaei, M.; Salimi, A. R.; Eshtiagh-Hosseini, H.

*Synthesis, X-Ray Characterization and Molecular Structure of a Novel Supramolecular Compound of Antimony(III); Theoretical Investigation on Molecular and Electronic Properties Based on the ab initio HF and Various DFT Methods*

Journal of the Iranian Chemical Society, (7): 500-509 2010.

Aghabozorg, H.; Motieyan, E.; Salimi, A. R.; Mirzaei, M.; Manteghi, F.; Shokrollahi, A.; Derki, S.; Ghadermazi, M.; Sheshmani, S.; Eshtiagh-Hosseini, H.

*Piperazinedium, Zr(IV) and Ce(IV) pyridine-2,6-dicarboxylates: Syntheses, characterizations, crystal structures, ab initio HF, DFT calculations and solution studies*  
Polyhedron, (29): 1453-1464 2010.

Aginagalde, M.; Vara, Y.; Arrieta, A.; Zangi, R.; Cebolla, V. L.; Delgado-Camon, A.; Cossio, F. P.

*Tandem [8+2] Cycloaddition-[2+6+2] Dehydrogenation Reactions Involving Imidazo[1,2-a]pyridines and Imidazo[1,2-a]pyrimidines*  
Journal of Organic Chemistry, (75): 2776-2784 2010.

Ahmadi, M. S.; Fattah, A.

*Dft Study on Metal Cationization and O-6-Protonation on 2'-Deoxyguanosine Configuration: Changes on Sugar Puckering and Strength of the N-Glycosidic Bond*  
Journal of Theoretical & Computational Chemistry, (9): 585-609 2010.

Alajarin, M.; Bonillo, B.; Sanchez-Andrade, P.; Vidal, A.

*Tandem 1,5-Hydride Shift/1,5-S,N-Cyclization with Ethylene Extrusion of 1,3-Oxathiolane-Substituted Ketenimines and Carbodiimides. An Experimental and Computational Study*  
Journal of Organic Chemistry, (75): 3737-3750 2010.

Alarcon, E.; Gonzalez-Bejar, M.; Gorelsky, S.; Ebensperger, R.; Lopez-Alarcon, C.; Carlos Netto-Ferreira, J.; Scaiano, J. C.

*Photophysical characterization of atorvastatin (Lipitor (R)) ortho-hydroxy metabolite: role of hydroxyl group on the drug photochemistry*  
Photochemical & Photobiological Sciences, (9): 1378-1384 2010.

Alary, F.; Heully, J.-L.; Scemama, A.; Garreau-de Bonneval, B.; Chane-Ching, K. I.; Caffarel, M.

*Structural and optical properties of a neutral Nickel bisdithiolene complex: density functional versus ab initio methods*

Theoretical Chemistry Accounts, (126): 243-255 2010.

Alberto, M. E.; Mazzone, G.; Russo, N.; Sicilia, E.

*The mutual influence of non-covalent interactions in pi-electron deficient cavities: the case of anion recognition by tetraoxacalix[2]arene[2]triazine*  
Chemical Communications, (46): 5894-5896 2010.

Alcaraz, G.; Chaplin, A. B.; Stevens, C. J.; Clot, E.; Vendier, L.; Weller, A. S.; Sabo-Etienne, S.

*Ruthenium, Rhodium, and Iridium Bis(sigma-B-H) Diisopropylaminoborane Complexes*  
Organometallics, (29): 5591-5595 2010.

Alcolea Palafox, M.; Rastogi, V. K.; Guerrero-Martinez, A.; Tardajos, G.; Joe, H.; Vats, J. K.

*Simulation of a tetramer form of 5-iodouracil: The vibrational spectra and molecular structure in the isolated and in the solid state by using DFT calculations*  
Vibrational Spectroscopy, (52): 108-121 2010.

Alcolea Palafox, M.; Talaya, J.  
*Hydration Analysis of Antiviral Agent AZT by Means of DFT and MP2 Calculations*  
Journal of Physical Chemistry B, (114): 15199-15211 2010.

Alexandrova, A. N.  
*H center dot(H<sub>2</sub>O)(n) Clusters: Microsolvation of the Hydrogen Atom via Molecular ab Initio Gradient Embedded Genetic Algorithm (GEGA)*  
Journal of Physical Chemistry A, (114): 12591-12599 2010.

Alexandrova, A. N.  
*Promiscuous DNA alkyladenine glycosylase dramatically favors a bound lesion over undamaged adenine*  
Biophysical Chemistry, (152): 118-127 2010.

Alkorta, I.; Blanco, F.; Elguero, J.  
*Dihydrogen Bond Cooperativity in Aza-borane Derivatives*  
Journal of Physical Chemistry A, (114): 8457-8462 2010.

Alkorta, I.; Blanco, F.; Elguero, J.; Schroeder, D.  
*Distinction between homochiral and heterochiral dimers of 1-aza[n]helicenes (n=1-7) with alkaline cations*  
Tetrahedron-Asymmetry, (21): 962-968 2010.

Alkorta, I.; Elguero, J.; Del Bene, J. E.; Mo, O.; Yanez, M.  
*New Insights into Factors Influencing B-N Bonding in X:BH<sub>3</sub>-nFn and X:BH<sub>3</sub>-nCl<sub>n</sub> for X = N-2, HCN, LiCN, H<sub>2</sub>CNH, NF<sub>3</sub>, NH<sub>3</sub> and n = 0-3: The Importance of Deformation*  
Chemistry-a European Journal, (16): 11897-11905 2010.

Alonso, M.; Angeles Alvarez, M.; Esther Garcia, M.; Garcia-Vivo, D.; Ruiz, M. A.  
*Chemistry of the Oxophosphinidene Ligand. 1. Electronic Structure of the Anionic Complexes [MCp{P(O)R\*}(CO)(2)](-) (M = Mo, W; R\* = 2,4,6-(C<sub>6</sub>H<sub>2</sub>Bu<sub>3</sub>)-Bu-t) and Their Reactions with H+ and C-Based Electrophiles*  
Inorganic Chemistry, (49): 8962-8976 2010.

Alvarez, M. A.; Amor, I.; Garcia, M. E.; Garcia-Vivo, D.; Ruiz, M. A.; Suarez, J.  
*Structure, Bonding, and Reactivity of Binuclear Complexes Having Asymmetric Trigonal Phosphinidene Bridges: Addition of 16-Electron Metal Carbonyl Fragments to the Dimolybdenum Compounds [Mo<sub>2</sub>Cp(mu-kappa(1):kappa(1),eta(5)-PC<sub>5</sub>H<sub>4</sub>)(CO)(2)L] and [Mo<sub>2</sub>Cp<sub>2</sub>(mu-PH)(CO)(2)L] (L = eta(6)-1,3,5-(C<sub>6</sub>H<sub>3</sub>Bu<sub>3</sub>)-Bu-t)*  
Organometallics, (29): 4384-4395 2010.

Amalanathan, M.; Joe, I. H.; Kostova, I.  
*Density functional theory calculation and vibrational spectral analysis of 4-hydroxy-3-(3-oxo-1-phenylbutyl)2H-1-benzopyran-2-one*

Journal of Raman Spectroscopy, (41): 1076-1084 2010.

Amalanathan, M.; Joe, I. H.; Prabhu, S. S.

*Charge Transfer Interaction and Terahertz Studies of a Nonlinear Optical Material L-Glutamine Picrate: A DFT Study*

Journal of Physical Chemistry A, (114): 13055-13064 2010.

Amar, A.; Meghezzi, H.; Boucekkine, A.; Kaoua, R.; Kolli, B.

*How to drive imine-enamine tautomerism of pyrronic derivatives of biological interest - A theoretical and experimental study of substituent and solvent effects*

Comptes Rendus Chimie, (13): 553-560 2010.

Ammal, S. C.; Heyden, A.

*Modeling the noble metal/TiO<sub>2</sub> (110) interface with hybrid DFT functionals: A periodic electrostatic embedded cluster model study*

Journal of Chemical Physics, (133) 2010.

An, X.; Jing, B.; Li, Q.

*Novel Halogen-Bonded Complexes H<sub>3</sub>NBH<sub>3</sub> center dot center dot center dot XY (XY = ClF, ClCl, BrF, BrCl, and BrBr): Partially Covalent Character*

Journal of Physical Chemistry A, (114): 6438-6443 2010.

Ando, K.

*The axial methionine ligand may control the redox reorganizations in the active site of blue copper proteins*

Journal of Chemical Physics, (133) 2010.

Aparicio, S.

*A Systematic Computational Study on Flavonoids*

International Journal of Molecular Sciences, (11): 2017-2038 2010.

Arago, J.; Viruela, P. M.; Orti, E.; Osuna, R. M.; Vercelli, B.; Zotti, G.; Hernandez, V.; Lopez Navarrete, J. T.; Henssler, J. T.; Matzger, A. J.; Suzuki, Y.; Yamaguchi, S.

*Neutral and Oxidized Triisopropylsilyl End-Capped Oligothienoacenes: A Combined Electrochemical, Spectroscopic, and Theoretical Study*

Chemistry-a European Journal, (16): 5481-5491 2010.

Arlund, D.; Micha, D. A.; Kilin, D. S.

*Computational Studies of the Optical Properties of Silicon Compounds Bonding to Silver Atoms and With Group III and V Substituents*

International Journal of Quantum Chemistry, (110): 3086-3094 2010.

Arnold, P. L.; Turner, Z. R.; Kaltsoyannis, N.; Pelekanaki, P.; Bellabarba, R. M.; Tooze, R. P.

*Covalency in Ce-IV and U-IV Halide and N-Heterocyclic Carbene Bonds*

Chemistry-a European Journal, (16): 9623-9629 2010.

Arnold, T.; Braunschweig, H.; Gross, M.; Kaupp, M.; Mueller, R.; Radacki, K.

*Electronic Structure and Reactivity of a [1],[1]Disilamolybdenocenophane*

Chemistry-a European Journal, (16): 3014-3020 2010.

Atsumi, T.; Abe, T.; Akiba, K.; Nakai, H.

*Theoretical Study of Bond-Switching in 1,6-Dihydro-6a-thia-1,6-diazapentalene (10-S-3) Systems Compared with Corresponding Oxygen Analogues*

Bulletin of the Chemical Society of Japan, (83): 520-529 2010.

Atsumi, T.; Abe, T.; Akiba, K.-y.; Nakai, H.

*Theoretical Study of Bond-Switching in 1,6-Dihydro-6a-thia-1,6-diazapentalene (10-S-3) Systems Compared with Corresponding Oxygen Analogues*

Bulletin of the Chemical Society of Japan, (83): 520-529 2010.

Attygalle, A. B.; Chan, C.-C.; Axe, F. U.; Bolgar, M.

*Generation of gas-phase sodiated arenes such as [(Na-3(C<sub>6</sub>H<sub>4</sub>)(+)] from benzene dicarboxylate salts*

Journal of Mass Spectrometry, (45): 72-81 2010.

Aucar, G. A.; Romero, R. H.; Maldonado, A. F.

*Polarization propagators: A powerful theoretical tool for a deeper understanding of NMR spectroscopic parameters*

International Reviews in Physical Chemistry, (29): 1-64 2010.

Autschbach, J.; Zheng, S.; Schurko, R. W.

*Analysis of Electric Field Gradient Tensors at Quadrupolar Nuclei in Common Structural Motifs*

Concepts in Magnetic Resonance Part A, (36A): 84-126 2010.

Averkiev, B. B.; Zhao, Y.; Truhlar, D. G.

*Binding energy of d(10) transition metals to alkenes by wave function theory and density functional theory*

Journal of Molecular Catalysis a-Chemical, (324): 80-88 2010.

Aydin, M.; Akins, D. L.

*Calculated dependence of vibrational band frequencies of single-walled and double-walled carbon nanotubes on diameter*

Vibrational Spectroscopy, (53): 163-172 2010.

Ayyappan, S.; Sundaraganesan, N.; Kurt, M.; Sertbakan, T. R.; Ozdur, M.

*Molecular structure, vibrational spectroscopic studies and NBO analysis of the 3,5-dichlorophenylboronic acid molecule by the density functional method*

Journal of Raman Spectroscopy, (41): 1379-1387 2010.

Azami, S. M.

*Electron Density Based Characterization of pi Bonds in Planar Molecules*

Journal of Physical Chemistry A, (114): 11794-11797 2010.

Azami, S. M.; Pooladi, R.; Setoudeh, N.

*Resonance structures might correspond to excited states in polycyclic conjugated systems*

Chemical Physics Letters, (491): 20-22 2010.

- Bachrach, S. M.; Wilbanks, C. C.  
*Using the Pyridine and Quinuclidine Scaffolds for Superbases: A DFT Study*  
Journal of Organic Chemistry, (75): 2651-2660 2010.
- Back, O.; Celik, M. A.; Frenking, G.; Melaimi, M.; Donnadieu, B.; Bertrand, G.  
*A Crystalline Phosphinyl Radical Cation*  
Journal of the American Chemical Society, (132): 10262-10263 2010.
- Back, O.; Donnadieu, B.; Parameswaran, P.; Frenking, G.; Bertrand, G.  
*Isolation of crystalline carbene-stabilized P-2-radical cations and P-2-dications*  
Nature Chemistry, (2): 369-373 2010.
- Backtorp, C.; Norrby, P.-O.  
*Trans effects in the Heck reaction-A model study*  
Journal of Molecular Catalysis a-Chemical, (328): 108-113 2010.
- Bakalbassis, E. G.; Malamidou-Xenikaki, E.; Spyroudis, S.; Xantheas, S. S.  
*Dimerization of Indanedioneketene to Spiro-oxetanone: A Theoretical Study*  
Journal of Organic Chemistry, (75): 5499-5504 2010.
- Bakker, H. J.; Skinner, J. L.  
*Vibrational Spectroscopy as a Probe of Structure and Dynamics in Liquid Water*  
Chemical Reviews, (110): 1498-1517 2010.
- Bandyopadhyay, R.; Cooper, B. F. T.; Rossini, A. J.; Schurko, R. W.; Macdonald, C. L. B.  
*Crown ether complexes of tin(II) trifluoromethanesulfonate*  
Journal of Organometallic Chemistry, (695): 1012-1018 2010.
- Banerjee, S.; Sengupta, P. S.; Mukherjee, A. K.  
*trans-Platinum anticancer drug AMD443: A detailed theoretical study by DFT-TST method on the hydrolysis mechanism*  
Chemical Physics Letters, (497): 142-148 2010.
- Banister, S. D.; Moussa, I. A.; Jordan, M. J. T.; Coster, M. J.; Kassiou, M.  
*Oxo-bridged isomers of aza-trishomocubane sigma (sigma) receptor ligands: Synthesis, in vitro binding, and molecular modeling*  
Bioorganic & Medicinal Chemistry Letters, (20): 145-148 2010.
- Bankiewicz, B.; Wojtulewski, S.; Grabowski, S. J.  
*Intramolecular Double Proton Transfer from 2-Hydroxy-2-iminoacetic Acid to 2-Amino-2-oxoacetic Acid*  
Journal of Organic Chemistry, (75): 1419-1426 2010.
- Banks, H. D.  
*Torquoselectivity Studies in the Generation of Azomethine Ylides from Substituted Aziridines*  
Journal of Organic Chemistry, (75): 2510-2517 2010.

- Bao, P.; Yu, Z.-H.  
*Restricted geometry optimization for estimating stabilization energies of polycyclic aromatic hydrocarbons*  
Journal of Physical Organic Chemistry, (23): 16-29 2010.
- Bao, X.; von Deak, D.; Biddinger, E. J.; Ozkan, U. S.; Hadad, C. M.  
*A computational exploration of the oxygen reduction reaction over a carbon catalyst containing a phosphinate functional group*  
Chemical Communications, (46): 8621-8623 2010.
- Baran, J. D.; Larsson, J. A.  
*Inversion of the shuttlecock shaped metal phthalocyanines MPc (M = Ge, Sn, Pb)-a density functional study*  
Physical Chemistry Chemical Physics, (12): 6179-6186 2010.
- Barreto, P. R. P.; Palazzetti, F.; Grossi, G.; Lombardi, A.; Maciel, G. S.; Vilela, A. F. A.  
*Range and Strength of Intermolecular Forces for van der Waals Complexes of the Type H<sub>2</sub>X<sub>n</sub>-Rg, With X = O, S and n=1, 2*  
International Journal of Quantum Chemistry, (110): 777-786 2010.
- Bartlett, G. J.; Choudhary, A.; Raines, R. T.; Woolfson, D. N.  
*n -> pi\* interactions in proteins*  
Nature Chemical Biology, (6): 615-620 2010.
- Baskaran, S.; Sivasankar, C.  
*Functionalization of Dinitrogen Using a Historically Significant Ru Complex: A New Life for an Old Complex*  
European Journal of Inorganic Chemistry: 4716-4719 2010.
- Bauer, J.; Braunschweig, H.; Brenner, P.; Kraft, K.; Radacki, K.; Schwab, K.  
*Late-Transition-Metal Complexes as Tunable Lewis Bases*  
Chemistry-a European Journal, (16): 11985-11992 2010.
- Bavafa, S.; Behjatmanesh-Ardakani, R.; Mashhadi, F. F.  
*Density functional study of the nitrosamine-formic acid and nitrosamine-formamide interactions*  
Journal of Molecular Structure-Theochem, (960): 15-21 2010.
- Bayse, C. A.; Rafferty, E. R.  
*Is Halogen Bonding the Basis for Iodothyronine Deiodinase Activity?*  
Inorganic Chemistry, (49): 5365-5367 2010.
- Bedeckovits, A.; Kollar, L.; Kegl, T.  
*Mechanistic investigation of platinum-catalysed hydroformylation of propene: A density functional study*  
Inorganica Chimica Acta, (363): 2029-2045 2010.
- Beheshtian, J.; Behzadi, H.; Esrafilii, M. D.; Shirvani, B. B.; Hadipour, N. L.  
*A computational study of water adsorption on boron nitride nanotube*

Structural Chemistry, (21): 903-908 2010.

Belpassi, L.; Reca, M. L.; Tarantelli, F.; Roncaratti, L. F.; Pirani, F.; Cappelletti, D.; Faure, A.; Scribano, Y.  
*Charge-Transfer Energy in the Water-Hydrogen Molecular Aggregate Revealed by Molecular-Beam Scattering Experiments, Charge Displacement Analysis, and ab Initio Calculations*  
Journal of the American Chemical Society, (132): 13046-13058 2010.

Belyakov, A. V.; Khramov, A. N.; Naumov, V. A.

*Molecular structure and conformational preferences of methylthiodichlorophosphite, Cl2PSCH3, as studied by gas electron diffraction and quantum-chemical calculations*  
Journal of Molecular Structure, (978): 4-10 2010.

Belyakov, A. V.; Khramov, A. N.; Naumov, V. N.

*Molecular Structure and Conformational Preferences of Gaseous Methylthiodichlorophosphite, Br2PSCH3, Studied by Gas Electron Diffraction and Quantum-Chemical Calculations*  
Russian Journal of General Chemistry, (80): 2249-2258 2010.

Ben Altabef, A.; Brandan, S. A.

*A new vibrational study of chromyl fluorosulfate, CrO2(SO3F)(2) by DFT calculations*  
Journal of Molecular Structure, (981): 146-152 2010.

Benidar, A.; Georges, R.; Guillemin, J.-C.; Mo, O.; Yanez, M.

*Infrared Spectra of a Species of Potential Prebiotic and Astrochemical Interest: Cyanoethenethiol (NC-CH=CH-SH)*  
Journal of Physical Chemistry A, (114): 9583-9588 2010.

Benn, M. H.; Huang, Y. Y.; Johannsen, F.; O'Reilly, M.; Parvez, M.; Rauk, A.; Sorensen, T.

*Concerning the conformational preferences of the 2-cyano derivatives of oxane, thiane, and selenane*

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 831-838 2010.

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

*Theoretical study of Z isomers of A-type dimeric proanthocyanidins substituted with R=H, OH and OCH3: stability and reactivity properties*  
Journal of Molecular Modeling, (16): 1895-1909 2010.

Bezbaruah, B.; Das, M. L.; Sarma, R. L.; Karim, M.; Medhi, C.

*Ab initio study on the nature of stacking between azaacridine-4-carboxamides with base pairs of DNA*  
Journal of Molecular Structure-Theochem, (947): 107-114 2010.

Bichara, L. C.; Lanus, H. E.; Nieto, C. G.; Brandan, S. A.

*Density Functional Theory Calculations of the Molecular Force Field of L-Ascorbic Acid, Vitamin C*  
Journal of Physical Chemistry A, (114): 4997-5004 2010.

Billes, F.; Holmgren, A.; Mikosch, H.

*A combined DFT and vibrational spectroscopy study of the nickel and zinc O,O-diethyldithiophosphate complexes*

Vibrational Spectroscopy, (53): 296-306 2010.

Biswal, H. S.; Shirhatti, P. R.; Wategaonkar, S.

*O-H center dot center dot center dot O versus O-H center dot center dot center dot S Hydrogen Bonding. 2. Alcohols and Thiols as Hydrogen Bond Acceptors*  
Journal of Physical Chemistry A, (114): 6944-6955 2010.

Biswal, H. S.; Wategaonkar, S.

*O-H center dot center dot center dot O versus O-H center dot center dot center dot S Hydrogen Bonding. 3. IR-UV Double Resonance Study of Hydrogen Bonded Complexes of p-Cresol with Diethyl Ether and Its Sulfur Analog*  
Journal of Physical Chemistry A, (114): 5947-5957 2010.

Blakemore, J. D.; Schley, N. D.; Balcells, D.; Hull, J. F.; Olack, G. W.; Incarvito, C. D.; Eisenstein, O.; Brudvig, G. W.; Crabtree, R. H.

*Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis*  
Journal of the American Chemical Society, (132): 16017-16029 2010.

Blanco, F.; Alkorta, I.; Rozas, I.; Elguero, J.

*Chiral recognition in self-complexes of diketopiperazine derivatives*  
Journal of Physical Organic Chemistry, (23): 1155-1172 2010.

Blanco, S.; Lopez, J. C.; Mata, S.; Alonso, J. L.

*Conformations of gamma-Aminobutyric Acid (GABA): The Role of the n ->pi Interaction*  
Angewandte Chemie-International Edition, (49): 9187-9192 2010.

Boerner, J.; Floerke, U.; Gloege, T.; Bannenberg, T.; Tamm, M.; Jones, M. D.; Doering, A.; Kuckling, D.; Herres-Pawlis, S.

*New insights into the lactide polymerisation with neutral N-donor stabilised zinc complexes: Comparison of imidazolin-2-imine vs. guanidine complexes*  
Journal of Molecular Catalysis a-Chemical, (316): 139-145 2010.

Bogatko, S.; Moens, J.; Geerlings, P.

*Cooperativity in Al3+ Hydrolysis Reactions from Density Functional Theory Calculations*  
Journal of Physical Chemistry A, (114): 7791-7799 2010.

Bonge, H. T.; Hansen, T.

*Computational comparison of Rh-2(esp)(2) and Rh-2(O2CH)(4) as catalysts in a carbenoid reaction*  
Tetrahedron Letters, (51): 5298-5301 2010.

Bonge, H. T.; Hansen, T.

*Computational Study of C-H Insertion Reactions with Ethyl Bromodiazoacetate*  
European Journal of Organic Chemistry: 4355-4359 2010.

Bonge, H. T.; Hansen, T.

*Computational Study of Cyclopropanation Reactions with Halodiazoacetates*  
Journal of Organic Chemistry, (75): 2309-2320 2010.

- Bonge, H. T.; Hansen, T.  
*Insights on Rh(II) carbenoid reactivity*  
Tetrahedron Letters, (51): 5378-5381 2010.
- Bonnet, S.; Siegler, M. A.; van Lenthe, J. H.; Lutz, M.; Spek, A. L.; van Koten, G.; Gebbink, R. J. M. K.  
*Ruthenium-to-Platinum Interactions in eta(6),eta(1) NCN-Pincer Arene Heterobimetallic Complexes: An Experimental and Theoretical Study*  
European Journal of Inorganic Chemistry: 4667-4677 2010.
- Boshra, A.; Monajjemi, M.; Aghaie, M.; Aghaie, H.  
*Density Functional Theory Investigation of Natural Bond Orbital Population Analysis and Gauge-Including Atomic Orbital NMR Tensors of K@B36N36*  
Journal of Computational and Theoretical Nanoscience, (7): 1147-1158 2010.
- Boyarskaya, I. A.; Akopian, S. K.  
*Spectroscopic Characteristics of Dimethylsulfoxide Molecules Coordinated to Mg<sup>2+</sup> Cation. Structure of Complexes [Mg(DMSO)(i)(CH<sub>3</sub>CN)(6-i)](2+) from the Data of Quantum-Chemical Calculations and IR Spectra of Mg(ClO<sub>4</sub>)<sub>2</sub>-DMSO-CH<sub>3</sub>CN Solutions*  
Russian Journal of General Chemistry, (80): 1296-1308 2010.
- Brandan, S. A.; Marquez Lopez, F.; Montejo, M.; Lopez Gonzalez, J. J.; Ben Altabef, A.  
*Theoretical and experimental vibrational spectrum study of 4-hydroxybenzoic acid as monomer and dimer*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (75): 1422-1434 2010.
- Bras, N. F.; Ramos, M. J.; Fernandes, P. A.  
*DFT studies on the beta-glycosidase catalytic mechanism: The deglycosylation step*  
Journal of Molecular Structure-Theochem, (946): 125-133 2010.
- Brock, D. S.; de Pury, J. J. C.; Mercier, H. P. A.; Schrobilgen, G. J.; Silvi, B.  
*A Rare Example of a Krypton Difluoride Coordination Compound: BrOF<sub>2</sub> AsF<sub>6</sub> center dot 2KrF(2)*  
Journal of the American Chemical Society, (132): 3533-3542 2010.
- Brock, D. S.; de Pury, J. J. C.; Mercier, H. P. A.; Schrobilgen, G. J.; Silvi, B.  
*XeF<sub>2</sub> Coordination to a Halogen Center; Raman Spectra (n=1, 2) and X-ray Crystal Structures (n=2) of [BrOF<sub>2</sub>][AsF<sub>6</sub>] center dot nXeF(2) and [XOF<sub>2</sub>][AsF<sub>6</sub>] (X = Cl, Br)*  
Inorganic Chemistry, (49): 6673-6689 2010.
- Brock, D. S.; Mercier, H. P. A.; Schrobilgen, G. J.  
*XeOF<sub>3</sub>-, an Example of an AX(3)YE(2) Valence Shell Electron Pair Repulsion Arrangement; Syntheses and Structural Characterizations of [M][XeOF<sub>3</sub>] (M = Cs, N(CH<sub>3</sub>)<sub>4</sub>)*  
Journal of the American Chemical Society, (132): 10935-10943 2010.
- Bruessel, M.; Zahn, S.; Hey-Hawkins, E.; Kirchner, B.  
*THEORETICAL INVESTIGATION OF SOLVENT EFFECTS AND COMPLEX SYSTEMS Toward the calculations of bioinorganic systems from ab initio molecular dynamics simulations and static quantum chemistry*

Advances in Inorganic Chemistry: Theoretical and Computational Inorganic Chemistry, Vol 62, (62): 111-142 2010.

Buchanan, W. D.; Allis, D. G.; Ruhlandt-Senge, K.

*Synthesis and stabilization-advances in organoalkaline earth metal chemistry*  
Chemical Communications, (46): 4449-4465 2010.

Buergel, C.; Mitric, R.; Bonacic-Koutecky, V.

*Theoretical study of structural and optical properties of small silver and gold clusters at defect centers of MgO*  
Physica Status Solidi B-Basic Solid State Physics, (247): 1099-1108 2010.

Buissonneaud, D. Y.; van Mourik, T.; O'Hagan, D.

*A DFT study on the origin of the fluorine gauche effect in substituted fluoroethanes*  
Tetrahedron, (66): 2196-2202 2010.

Burkhardt, S. E.; Rodriguez-Calero, G. G.; Lowe, M. A.; Kiya, Y.; Hennig, R. G.; Abruna, H. D.

*Theoretical and Electrochemical Analysis of Poly(3,4-alkylenedioxythiophenes): Electron-Donating Effects and Onset of p-Doped Conductivity*  
Journal of Physical Chemistry C, (114): 16776-16784 2010.

Butler, M.; Arroyo Manez, P.; Cabrera, G. M.

*An experimental and computational study on the dissociation behavior of hydroxypyridine N-oxides in atmospheric pressure ionization mass spectrometry*  
Journal of Mass Spectrometry, (45): 536-544 2010.

Butschies, M.; Sauer, S.; Kessler, E.; Siehl, H.-U.; Claasen, B.; Fischer, P.; Frey, W.; Laschat, S.

*Influence of N-Alkyl Substituents and Counterions on the Structural and Mesomorphic Properties of Guanidinium Salts: Experiment and Quantum Chemical Calculations*  
Chemphyschem, (11): 3752-3765 2010.

Cabeza, J. A.; del Rio, I.; Perez-Carreno, E.; Gabriela Sanchez-Vega, M.; Vazquez-Garcia, D.

*Trapping of Pyrid-2-ylidenes by [Ru-3(CO)(12)]: Orthometalated Pyrid-2-ylidenes in Triruthenium Clusters*  
Organometallics, (29): 4464-4471 2010.

Cabeza, J. A.; del Rio, I.; Perez-Carreno, E.; Pruneda, V.

*Reductive Dimerization of Triruthenium Clusters Containing Cationic Aromatic N-Heterocyclic Ligands*  
Chemistry-a European Journal, (16): 5425-5436 2010.

Cai, W.; Wu, H.; Wang, X.; Li, L.; Tian, A.; Wong, N.

*Density Functional Theory Study of the Interaction between Guanine and Catechin*  
Chinese Journal of Chemistry, (28): 2137-2143 2010.

Camacho, R. L.; Montiel, E.; Jayanthi, N.; Pandiyan, T.; Cruz, J.

*DFT studies of alpha-diimines adsorption over Fe-n surface (n=1, 4, 9 and 14) as a model for metal surface coating*

Chemical Physics Letters, (485): 142-151 2010.

Candeias, N. R.; Cal, P. M. S. D.; Andre, V.; Duarte, M. T.; Veiros, L. F.; Gois, P. M. P.

*Water as the reaction medium for multicomponent reactions based on boronic acids*  
Tetrahedron, (66): 2736-2745 2010.

Cannon, J. S.; Kirsch, S. F.; Overman, L. E.; Sneddon, H. F.

*Mechanism of the Cobalt Oxazoline Palladacycle (COP)-Catalyzed Asymmetric Synthesis of Allylic Esters*

Journal of the American Chemical Society, (132): 15192-15203 2010.

Canotilho, J.; Castro, R. A. E.

*The structure of betaxolol studied by infrared spectroscopy and natural bond orbital theory*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (76): 395-400 2010.

Cao, D.-L.; Zhang, W.-Y.; Ren, F.-D.; Hou, S.-Q.

*Density Functional Theory Studies on the Intermolecular Interactions of Five Aza-calix[6]arene Host with HMX*  
Chinese Journal of Structural Chemistry, (29): 377-384 2010.

Cao, L. J.; Li, A. Y.; Ji, H. B.; Xu, L.; Zhang, Y.

*Theoretical study on the ring stretching modes of pyridine in the hydrogen bonding with H<sub>2</sub>O, HCONH<sub>2</sub> and CH<sub>3</sub>COOH*

Journal of Molecular Structure-Theochem, (959): 80-86 2010.

Cao, L.-J.; Ai, H.-Q.; Zheng, L.-M.; Wang, S.-N.; Zhou, M.-J.; Liu, J.-F.; Zhang, C.

*Theoretical study on the interaction of neutral and charged Ti-n (n=1-7) clusters with one nitrogen molecule*

Journal of Molecular Structure-Theochem, (948): 65-70 2010.

Cao, X.; Qin, S.; Su, Z.; Yang, H.; Hu, C.; Feng, X.

*Theoretical Study on Hetero-Diels-Alder Reaction of Butadiene with Benzaldehyde Catalyzed by Chiral In-III Complexes*

European Journal of Organic Chemistry: 3867-3875 2010.

Carrera, E. M.; Flores-Gallegos, N.; Esquivel, R. O.

*Natural atomic probabilities in quantum information theory*

Journal of Computational and Applied Mathematics, (233): 1483-1490 2010.

Castro, L.; Lam, O. P.; Bart, S. C.; Meyer, K.; Maron, L.

*Carbonate Formation from CO<sub>2</sub> via Oxo versus Oxalate Pathway: Theoretical Investigations into the Mechanism of Uranium-Mediated Carbonate Formation*

Organometallics, (29): 5504-5510 2010.

Castro, L.; Yahia, A.; Maron, L.

*A DFT study of the reactivity of actinidocenes (U, Np and Pu) with pyridine and pyridine N-oxide derivatives*

Dalton Transactions, (39): 6682-6692 2010.

Castro, L.; Yahia, A.; Maron, L.

*A DFT study of the reactivity of Cp(2)AnMe(2) with pyridine N-oxide: Towards a predicted different reactivity of U/Pu and Np*  
Comptes Rendus Chimie, (13): 870-875 2010.

Catak, S.; D'Hooghe, M.; De Kimpe, N.; Waroquier, M.; Van Speybroeck, V.

*Intramolecular pi-pi Stacking Interactions in 2-Substituted N,N-Dibenzylaziridinium Ions and Their Regioselectivity in Nucleophilic Ring-Opening Reactions*  
Journal of Organic Chemistry, (75): 885-896 2010.

Catak, S.; D'Hooghe, M.; Verstraelen, T.; Hemelsoet, K.; Van Nieuwenhove, A.; Ha, H.-J.; Waroquier, M.; De Kimpe, N.; Van Speybroeck, V.

*Opposite Regiospecific Ring Opening of 2-(Cyanomethyl)aziridines by Hydrogen Bromide and Benzyl Bromide: Experimental Study and Theoretical Rationalization*  
Journal of Organic Chemistry, (75): 4530-4541 2010.

Ceron-Carrasco, J. P.; Requena, A.; Perpete, E. A.; Michaux, C.; Jacquemin, D.

*Theoretical Study of the Tautomerism in the One-Electron Oxidized Guanine-Cytosine Base Pair*  
Journal of Physical Chemistry B, (114): 13439-13445 2010.

Chen, H.-p.; Ding, J.-n.; Yuan, N.-y.; Wang, X.-q.; Chen, C.-l.; Weng, D.

*First-principle study of interaction of H(2) and H(2)O molecules with (ZnO)(n)(n=3-6) ring clusters*  
Progress in Natural Science-Materials International, (20): 30-37 2010.

Chen, J. C.; Chen, L. M.; Liao, S. Y.; Zheng, K. C.; Ji, L. N.

*A DFT Study on the Hydrolysis Mechanism of NH-Tautomeric Antitumors of [HL][trans-RuCl4L(dmsO-S)]*  
International Journal of Quantum Chemistry, (110): 1252-1263 2010.

Chen, S.; Ma, J.

*The influence of orientations and external electric field on charge carrier mobilities in CuPc and F16CuPc films on highly ordered pyrolytic graphite and octane-1-thiol terminated Au(111) substrates*  
Physical Chemistry Chemical Physics, (12): 12177-12187 2010.

Chen, S. A.; Ma, J.

*The influence of orientations and external electric field on charge carrier mobilities in CuPc and F16CuPc films on highly ordered pyrolytic graphite and octane-1-thiol terminated Au(111) substrates*  
Physical Chemistry Chemical Physics, (12): 12177-12187 2010.

Chen, Y. K.; Liu, L. V.; Wang, Y. A.

*Density Functional Study of Interaction of Atomic Pt with Pristine and Stone-Wales-Defective Single-Walled Boron Nitride Nanotubes*  
Journal of Physical Chemistry C, (114): 12382-12388 2010.

Chen, Y. Z.; Tian, Y. H.; Kertesz, M.; Weiss, R. G.

*Why is there no in-plane H-atom transfer from aryloxy radicals? A theoretical and experimental investigation*

Photochemical & Photobiological Sciences, (9): 1203-1211 2010.

Chen, Y.-Z.; Tian, Y.-H.; Kertesz, M.; Weiss, R. G.

*Why is there no in-plane H-atom transfer from aryloxy radicals? A theoretical and experimental investigation*

Photochemical & Photobiological Sciences, (9): 1203-1211 2010.

Cheng, H.; Djukic, B.; Jenkins, H. A.; Gorelsky, S. I.; Lemaire, M. T.

*Iron(II) complexes containing thiophene-substituted "bispicen" ligands - Spin-crossover, ligand rearrangements, and ferromagnetic interactions*

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 954-963 2010.

Cheng, J.; Li, R.; Li, Q.; Jing, B.; Liu, Z.; Li, W.; Gong, B.; Sun, J.

*Prominent Effect of Alkali Metals in Halogen-Bonded Complex of MCCBr-NCM' (M and M' = H, Li, Na, F, NH<sub>2</sub>, and CH<sub>3</sub>)*

Journal of Physical Chemistry A, (114): 10320-10325 2010.

Cheng, Q.; Gu, J.; Compaan, K. R.; Schaefer, H. F., III

*Hydroxyl Radical Reactions with Adenine: Reactant Complexes, Transition States, and Product Complexes*

Chemistry-a European Journal, (16): 11848-11858 2010.

Chermahini, A. N.; Moaddeli, A.; Teimouri, A.

*Ab initio and DFT studies of hydrogen bond interactions in difluoroacetic acid dimer*

Structural Chemistry, (21): 643-649 2010.

Chimni, S. S.; Bala, N.; Dixit, V. A.; Bharatam, P. V.

*Thiourea catalyzed aminolysis of epoxides under solvent free conditions. Electronic control of regioselective ring opening*

Tetrahedron, (66): 3042-3049 2010.

Choudhary, A.; Fry, C. G.; Raines, R. T.

*Modulation of an n->pi\* interaction with alpha-fluoro groups*

Arkivoc: 251-262 2010.

Choudhary, A.; Kamer, K. J.; Powner, M. W.; Sutherland, J. D.; Raines, R. T.

*A Stereoelectronic Effect in Prebiotic Nucleotide Synthesis*

ACS Chemical Biology, (5): 655-657 2010.

Chowdhury, S.; Himo, F.; Russo, N.; Sicilia, E.

*Mechanistic Investigation of the Hydrogenation of O-2 by a Transfer Hydrogenation Catalyst*

Journal of the American Chemical Society, (132): 4178-4190 2010.

Chrostowska, A.; Dargelos, A.; Graciaa, A.

*UV-photoelectron Spectroscopy of Unhindered Germylenes and Carbon-arsenic Multiple-bonded Species*

Australian Journal of Chemistry, (63): 1608-1614 2010.

Chung, T. W.; Turecek, F.

*Backbone and Side-Chain Specific Dissociations of z Ions from Non-Tryptic Peptides*  
Journal of the American Society for Mass Spectrometry, (21): 1279-1295 2010.

Ciupka, J.; Cao-Dolg, X.; Wiebke, J.; Dolg, M.

*Computational study of lanthanide(III) hydration*

Physical Chemistry Chemical Physics, (12): 13215-13223 2010.

Clark, J.; Call, S. T.; Austin, D. E.; Hansen, J. C.

*Computational Study of Isoprene Hydroxylalkyl Peroxy Radical Water Complexes (C<sub>5</sub>H<sub>8</sub>(OH)O-2-H<sub>2</sub>O)*

Journal of Physical Chemistry A, (114): 6534-6541 2010.

Clark, T.

*The local electron affinity for non-minimal basis sets*

Journal of Molecular Modeling, (16): 1231-1238 2010.

Coll, C.; Aznar, E.; Martinez-Manez, R.; Dolores Marcos, M.; Sancenon, F.; Soto, J.; Amoros, P.; Cano, J.; Ruiz, E.

*Fatty Acid Carboxylate- and Anionic Surfactant-Controlled Delivery Systems That Use Mesoporous Silica Supports*

Chemistry-a European Journal, (16): 10048-10061 2010.

Conrad, A. R.; Barefoot, N. Z.; Tubergen, M. J.

*Rotational spectra of o-, m-, and p-cyanophenol and internal rotation of p-cyanophenol*

Physical Chemistry Chemical Physics, (12): 8350-8356 2010.

Contreras, R. H.; dos Santos, F. P.; Ducati, L. C.; Tormena, C. F.

*Difference between (2)J(C<sub>2</sub>H<sub>3</sub>) and (2)J(C<sub>3</sub>H<sub>2</sub>) spin-spin couplings in heterocyclic five- and six-membered rings as a probe for studying sigma-ring currents: a quantum chemical analysis*  
Magnetic Resonance in Chemistry, (48): S151-S158 2010.

Contreras, R. H.; Suardiaz, R.; Perez, C.; Crespo-Otero, R.; San Fabian, J.; Garcia De La Vega, J. M.

*NMR Spin-Spin Coupling Constants and Hyperconjugative Interactions*

International Journal of Quantum Chemistry, (110): 532-539 2010.

Coronel, A. C.; Fernandez, L. E.; Varetti, E. L.

*Scaled Quantum Mechanical Force Fields for the Peroxynitrates. II. Fluorocarbonyl Peroxynitrate and Chlorocarbonyl Peroxynitrate*

Zeitschrift fur Anorganische und Allgemeine Chemie, (636): 721-726 2010.

Cortes-Guzman, F.; Hernandez-Trujillo, J.; Cuevas, G.

*Application of the additivity of group energies to understand conformational preference: the anomeric effect*

Physical Chemistry Chemical Physics, (12): 13261-13265 2010.

Cremer, D.; Kraka, E.

*From Molecular Vibrations to Bonding, Chemical Reactions, and Reaction Mechanism*  
Current Organic Chemistry, (14): 1524-1560 2010.

Cremer, T.; Kolbeck, C.; Lovelock, K. R. J.; Paape, N.; Woelfel, R.; Schulz, P. S.; Wasserscheid, P.; Weber, H.; Thar, J.; Kirchner, B.; Maier, F.; Steinrueck, H.-P.

*Towards a Molecular Understanding of Cation-Anion Interactions-Probing the Electronic Structure of Imidazolium Ionic Liquids by NMR Spectroscopy, X-ray Photoelectron Spectroscopy and Theoretical Calculations*  
Chemistry-a European Journal, (16): 9018-9033 2010.

Cucarull-Gonzalez, J. R.; Hernando, J.; Alibes, R.; Figueredo, M.; Font, J.; Rodriguez-Santiago, L.; Sodupe, M.

*[2+2] Photocycloaddition of 2(5H)-Furanone to Unsaturated Compounds. Insights from First Principles Calculations and Transient-Absorption Measurements*  
Journal of Organic Chemistry, (75): 4392-4401 2010.

Cui, F.-C.; Pan, X.-L.; Liu, J.-Y.

*Catalytic Mechanism of Hydroxynitrile Lyase from Hevea brasiliensis: A Theoretical Investigation*  
Journal of Physical Chemistry B, (114): 9622-9628 2010.

Cui, Y. H.; Tian, W. Q.; Feng, J. K.; Chen, D. L.

*Structures, stabilities, aromaticity, and electronic properties of C-66 fullerene isomers, anions (C-66(2-), C-66(4-), C-66(6-)), and metallofullerenes (Sc-2@C-66)*  
Journal of Nanoparticle Research, (12): 429-438 2010.

Cui, Y.-H.; Tian, W. Q.; Feng, J.-K.; Chen, D.-L.

*Structures, stabilities, aromaticity, and electronic properties of C-66 fullerene isomers, anions (C-66(2-), C-66(4-), C-66(6-)), and metallofullerenes (Sc-2@C-66)*  
Journal of Nanoparticle Research, (12): 429-438 2010.

Cuypers, R.; Murali, S.; Marcelis, A. T. M.; Sudholter, E. J. R.; Zuilhof, H.

*Complexation of Phenol and Thiophenol by Amine N-Oxides: Isothermal Titration Calorimetry and ab Initio Calculations*  
Chemphyschem, (11): 3465-3473 2010.

Cuypers, R.; Sudholter, E. J. R.; Zuilhof, H.

*Hydrogen Bonding in Phosphine Oxide/Phosphate-Phenol Complexes*  
Chemphyschem, (11): 2230-2240 2010.

Cypyrek, M.; Delczyk-Olejniczak, B.

*Copolymerization of functional cyclotrisiloxanes - a reactivity comparison*  
Polimery, (55): 503-511 2010.

Dabbagh, H. A.; Rasti, E.; Le Grel, P.; Hocquet, A.

*DFT, ab initio, NMR, and NBO analyses of N-alpha-substituted hydrazino acetamides: Experimental vs theoretical values*  
Tetrahedron, (66): 2322-2330 2010.

- Dabbagh, H. A.; Zamani, M.; Farrokhpour, H.; Habibi, M. H.; Barati, K.  
*Conformational analysis and intramolecular/intermolecular interactions of N,N'-dibenzylideneethylenediamine derivatives*  
Journal of Molecular Structure, (983): 169-185 2010.
- Dabbagh, H. A.; Zamani, M.; Farrokhpour, H.; Namazian, M.; Habibabadi, H. E.  
*Influence of B, Ga and In impurities in the structure and electronic properties of alumina nanoball*  
Chemical Physics Letters, (485): 176-182 2010.
- Dai, G.-L.; Wang, C.-F.; Chen, H.; Wu, J.-Y.; Yan, H.; Zhong, A.-G.  
*Theoretical study on the reactions of Zr+ and Zr with CO<sub>2</sub> in gas phase*  
Russian Journal of Physical Chemistry A, (84): 2238-2246 2010.
- Dai, G.-L.; Wang, C.-F.; Jin, Y.-X.; Zhao, J.; Zhong, A.-G.; Han, D.-M.  
*Theoretical investigation of the reactions of La atom and La+ cation with carbonyl sulfide*  
Russian Journal of Physical Chemistry A, (84): 971-979 2010.
- Dakkouri, M.; Novikov, V. P.; Vilkov, L. V.  
*A gas-phase electron diffraction and quantum chemical investigation of the molecular structure of 1-bromosilacyclobutane*  
Journal of Molecular Structure, (978): 234-245 2010.
- Dakkouri, M.; Typke, V.  
*The molecular structure of 1,1-dichlorosilacyclopentane as obtained from gas-phase electron diffraction and ab initio calculations*  
Journal of Molecular Structure, (978): 48-60 2010.
- Das, S.; Dutta, P. K.; Panda, S.; Zade, S. S.  
*3,4-Ethylenedioxythiophene and 3,4-Ethylenedioxysephenophene: Synthesis and Reactivity of C-alpha-Si Bond*  
Journal of Organic Chemistry, (75): 4868-4871 2010.
- Dash, C.; Shaikh, M. M.; Butcher, R. J.; Ghosh, P.  
*A comparison between nickel and palladium precatalysts of 1,2,4-triazole based N-heterocyclic carbenes in hydroamination of activated olefins*  
Dalton Transactions, (39): 2515-2524 2010.
- Dash, C.; Shaikh, M. M.; Butcher, R. J.; Ghosh, P.  
*Highly Convenient Regioselective Intermolecular Hydroamination of Alkynes Yielding Ketimines Catalyzed by Gold(I) Complexes of 1,2,4-triazole Based N-heterocyclic Carbenes*  
Inorganic Chemistry, (49): 4972-4983 2010.
- Davari, M. D.; Bahrami, H.; Haghghi, Z. Z.; Zahedi, M.  
*Quantum chemical investigation of intramolecular thione-thiol tautomerism of 1,2,4-triazole-3-thione and its disubstituted derivatives*  
Journal of Molecular Modeling, (16): 841-855 2010.

Davari, M. D.; Bahrami, H.; Zahedi, M.; Safari, N.  
*Effect of the axial ligands on the structure and reactivity of tin verdoheme in the ring opening process*  
Inorganica Chimica Acta, (363): 1577-1586 2010.

David, C.; Enescu, M.  
*Free Energy Calculations on Disulfide Bridges Reduction in Proteins by Combining ab Initio and Molecular Mechanics Methods*  
Journal of Physical Chemistry B, (114): 3020-3027 2010.

Davidson, R. J.; Ainscough, E. W.; Brodie, A. M.; Harrison, J. A.; Waterland, M. R.  
*The Nature of the Phosphazene Nitrogen Metal Bond: DFT Calculations on 2-(Pyridyloxy)cyclophosphazene Complexes*  
European Journal of Inorganic Chemistry: 1619-1625 2010.

de Almeida, K. J.; Duarte, H. A.  
*Dehydrogenation of Methane by Gas-Phase Th, Th+, and Th2+: Theoretical Insights into Actinide Chemistry*  
Organometallics, (29): 3735-3745 2010.

De Vleeschouwer, F.; De Proft, F.; Geerlings, P.  
*Conceptual density functional theory based intrinsic radical stabilities: Application to substituted silylenes and p-benzynes*  
Journal of Molecular Structure-Theochem, (943): 94-102 2010.

De Vleeschouwer, F.; Jaque, P.; Geerlings, P.; Toro-Labbe, A.; De Proft, F.  
*Regioselectivity of Radical Additions to Substituted Alkenes: Insight from Conceptual Density Functional Theory*  
Journal of Organic Chemistry, (75): 4964-4974 2010.

Deakyne, C. A.; Ludden, A. K.; Victoria Roux, M.; Notario, R.; Demchenko, A. V.; Chickos, J. S.; Liebman, J. F.  
*Energetics of the Lighter Chalcogen Analogues of Carboxylic Acid Esters*  
Journal of Physical Chemistry B, (114): 16253-16262 2010.

Debnath, S.; Hausner, D. B.; Strongin, D. R.; Kubicki, J.  
*Reductive dissolution of ferrihydrite by ascorbic acid and the inhibiting effect of phospholipid*  
Journal of Colloid and Interface Science, (341): 215-223 2010.

Defonsi Lestard, M. E.; Eugenia Tuttolomondo, M.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.; Ben Altabef, A.  
*Experimental and theoretical structure and vibrational analysis of ethyl trifluoroacetate, CF<sub>3</sub>CO<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>*  
Journal of Raman Spectroscopy, (41): 1357-1368 2010.

Defonsi Lestard, M. E.; Tuttolomondo, M. E.; Varetti, E. L.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.; Ben Altabef, A.

*Investigation of the gas-phase structure and rotational barrier of trimethylsilyl trifluoromethanesulfonate and comparison with covalent sulfonates*  
Journal of Molecular Structure, (984): 376-382 2010.

Defonsi Lestard, M. E.; Tuttolomondo, M. E.; Varetti, E. L.; Warnn, D. A.; Robertson, H. E.; Rankin, D. W. H.; Ben Altabef, A.

*Gas-phase structure, rotational barrier and vibrational properties of trimethylsilyl trifluoroacetate CF<sub>3</sub>C(O)OSi(CH<sub>3</sub>)<sub>3</sub>: An experimental and computational study*  
Journal of Molecular Structure, (978): 114-123 2010.

Demir, S.; Lorenz, S. E.; Fang, M.; Furche, F.; Meyer, G.; Ziller, J. W.; Evans, W. J.  
*Synthesis, Structure, and Density Functional Theory Analysis of a Scandium Dinitrogen Complex, [(C<sub>5</sub>Me<sub>4</sub>H)(2)Sc](2)(mu-eta(2):eta(2)-N-2)*  
Journal of the American Chemical Society, (132): 11151-11158 2010.

Demir, S.; Yolcu, Z.; Andac, O.; Buyukgungor, O.; Yazicilar, T. K.  
*Electronic structure modeling of dinuclear copper(II)-methacrylic acid complex by density functional theory*  
Journal of Molecular Modeling, (16): 1509-1518 2010.

Dem'yanov, P. I.; Poleshchuk, P. M.; Gloriozov, I. P.; Vasil'kov, A. Y.  
*Intramolecular Noncovalent Interactions: Bis(toluene)chromium(0)Conformers*  
Russian Journal of Physical Chemistry A, (84): 1731-1744 2010.

Deng, C.; Zhou, L.  
*Binding of ansa- and non-ansa-titanocene anticancer drugs to DNA: a DFT study*  
Structural Chemistry, (21): 735-744 2010.

Dethlefsen, J. R.; Dossing, A.; Hedegard, E. D.  
*Electron Paramagnetic Resonance Studies of Nitrosyl and Thionitrosyl and Density Functional Theory Studies of Nitrido, Nitrosyl, Thionitrosyl, and Selenonitrosyl Complexes of Chromium*  
Inorganic Chemistry, (49): 8769-8778 2010.

Dhayal, R. S.; Sahoo, S.; Reddy, K. H. K.; Mobin, S. M.; Jemmis, E. D.; Ghosh, S.  
*Vertex-Fused Metallaborane Clusters: Synthesis, Characterization and Electronic Structure of [(eta(5)-C<sub>5</sub>Me<sub>5</sub>Mo)(3)MoB<sub>9</sub>H<sub>18</sub>]*  
Inorganic Chemistry, (49): 900-904 2010.

Diao, K. S.; Wang, F.; Wang, H. J.  
*Ab Initio Theoretical Study of the Interactions Between CFCI<sub>3</sub> and SO<sub>2</sub>*  
Bulletin of Environmental Contamination and Toxicology, (84): 170-174 2010.

Die, D.; Kuang, X.-Y.; Guo, J.-J.; Zheng, B.-X.  
*Density functional theory study of A<sub>n</sub>Mn(n=1-8) clusters*  
Journal of Physics and Chemistry of Solids, (71): 770-775 2010.

Die, D.; Kuang, X.-Y.; Guo, J.-J.; Zheng, B.-X.

*Geometries, stabilities, and magnetic properties of Cr@Au-n (n = 1-8) clusters: Density functional theory study*

Physica a-Statistical Mechanics and Its Applications, (389): 5216-5222 2010.

Dimitrova, Y.

*Theoretical study on the structure, stability and vibrational spectra of the hydrogen-bonded phenoxides, containing strong short hydrogen bonds*  
Bulgarian Chemical Communications, (42): 236-245 2010.

Ding, Y.; Feng, S.; Li, T. D.; Wang, Y.; Liu, Y.; Xue, L.; Wang, Y.; Wang, H.; Yue, Y.

*Theoretical study on a new kind of thietyl-functionalized polysilane*  
Structural Chemistry, (21): 1263-1271 2010.

Ding, Y.; Feng, S.; Sun, X.; Diao, S.; Yang, Z.; Xu, Q.; Liang, Y.; Wang, X.; Jin, K.

*The tunability of the electronic structures for poly(carbosilylsilanes): a theoretical study*  
Structural Chemistry, (21): 583-592 2010.

Ding, Y. Q.; Qiao, Q. A.; Wang, P.; Chen, G. W.; Han, J. J.; Xu, Q.; Feng, S. Y.

*A DFT study of electronic structures of thiophene-based organosilicon compounds*  
Chemical Physics, (367): 167-174 2010.

Ding, Y.-q.; Qiao, Q.-a.; Wang, P.; Chen, G.-w.; Han, J.-j.; Xu, Q.; Feng, S.-y.

*A DFT study of electronic structures of thiophene-based organosilicon compounds*  
Chemical Physics, (367): 167-174 2010.

Dinoi, C.; Ciclosi, M.; Manoury, E.; Maron, L.; Perrin, L.; Poli, R.

*Olefin Epoxidation by H<sub>2</sub>O<sub>2</sub>/MeCN Catalysed by Cyclopentadienyloxidotungsten(VI) and Molybdenum(VI) Complexes: Experiments and Computations*  
Chemistry-a European Journal, (16): 9572-9584 2010.

Dixit, V. A.; Rathi, P. C.; Bharatam, P. V.

*Intramolecular dihydrogen bond A new perspective in Lewis acid catalyzed nucleophilic epoxide ring opening reaction*  
Journal of Molecular Structure-Theochem, (962): 97-100 2010.

Dixon, I. M.; Alary, F.; Heully, J.-L.

*Electronic peculiarities of the excited states of [RuN<sub>5</sub>C](+) vs. [RuN<sub>6</sub>](2+) polypyridine complexes: insight from theory*  
Dalton Transactions, (39): 10959-10966 2010.

Djukic, J.-P.; Fetzer, L.; Czysz, A.; Iail, W.; Sirlin, C.; Pfeffer, M.

*One-Pot Generation of a Tris-cationic Homobimetallic Planar-Chiral Ruthenacycle*  
Organometallics, (29): 1675-1679 2010.

Domingo, L. R.; Aurell, M. J.; Jalal, R.; Esseffar, M.

*A DFT study of the role of the Mg complex formation on the mechanism of the 1,3-dipolar cycloadditions of benzonitrile oxides with acryloylpyrazolidinone*  
Journal of Molecular Structure-Theochem, (942): 26-31 2010.

- Domingo, L. R.; Chamorro, E.; Perez, P.  
*Understanding the High Reactivity of the Azomethine Ylides in [3+2] Cycloaddition Reactions*  
Letters in Organic Chemistry, (7): 432-439 2010.
- Domingo, L. R.; Chamorro, E.; Perez, P.  
*Understanding the mechanism of non-polar Diels-Alder reactions. A comparative ELF analysis of concerted and stepwise diradical mechanisms*  
Organic & Biomolecular Chemistry, (8): 5495-5504 2010.
- Domingo, L. R.; Jose Aurell, M.; Jalal, R.; Esseffar, M. h.  
*A DFT study of the role of the Mg complex formation on the mechanism of the 1,3-dipolar cycloadditions of benzonitrile oxides with acryloylpyrazolidinone*  
Journal of Molecular Structure-Theochem, (942): 26-31 2010.
- Domingo, L. R.; Zaragoza, R. J.; Arno, M.  
*Understanding the mechanism of stereoselective synthesis of cyclopentenes via N-heterocyclic carbene catalyzed reactions of enals with enones*  
Organic & Biomolecular Chemistry, (8): 4884-4891 2010.
- Dominguez, Z.; Hernandez, J.; Silva-Gutierrez, L.; Salas-Reyes, M.; Sanchez, M.; Merino, G.  
*Substituent Effects on  $^{31}\text{P}$  NMR Chemical Shifts and  $^{1}\text{JP-}\text{Se}$  of triarylselenophosphates*  
Phosphorus Sulfur and Silicon and the Related Elements, (185): 772-784 2010.
- Dominikowska, J.; Palusiak, M.  
*Cyclooctatetraene in metal complexes-planar does not mean aromatic*  
New Journal of Chemistry, (34): 1855-1861 2010.
- Donald, K. J.; Wittmaack, B. K.; Crigger, C.  
*Tuning sigma-Holes: Charge Redistribution in the Heavy (Group 14) Analogs of Simple and Mixed Halomethanes Can Impose Strong Propensities for Halogen Bonding*  
Journal of Physical Chemistry A, (114): 7213-7222 2010.
- Dong, C.; Yang, J.; Ning, H.; Li, C.  
*Studies on structures, energetics, and electron affinities of As-nucleobases and their anions with density functional theory*  
Journal of Molecular Structure-Theochem, (950): 64-71 2010.
- Dong, Q.; Li, X. M.; Tian, W. Q.; Huang, X.-R.; Sun, C.-C.  
*Theoretical studies on the adsorption of small molecules on Pt-doped BN nanotubes*  
Journal of Molecular Structure-Theochem, (948): 83-92 2010.
- Dong, Q.; Tian, W.-Q.; Li, W.-Q.; Sun, X.-D.; Sun, C.-C.  
*Effects of Electric Field on the Structures and Electronic Properties of N@C-60, P@C-60 and As@C-60*  
Chemical Journal of Chinese Universities-Chinese, (31): 2254-2259 2010.
- Dong, X.-f.; Ren, F.-d.; Cao, D.-l.; Wang, W.-n.; Zhang, F.-q.

*A MP2(full) theoretical investigation on the pi-halogen interaction between OCB BCO and X<sub>1</sub>X<sub>2</sub> (X<sub>1</sub>, X<sub>2</sub>=F, Cl, Br)*  
Journal of Molecular Structure-Theochem, (961): 73-82 2010.

Donoso, D.; Mendizabal, F.  
*Theoretical Study of the S-2-P Interaction between Tl(I) and Olefinic Systems on Hypothetical [Tl(C<sub>2</sub>h<sub>4</sub>)(2)](+) and [Tl(C<sub>2</sub>h<sub>2</sub>)(N)](+) (N=2,3) Complexes*  
Journal of the Chilean Chemical Society, (55): 503-505 2010.

Doronina, E. P.; Sidorkin, V. F.; Lazareva, N. F.  
*(PO -> Si) Chelates of Silylmethyl Derivatives of Phosphoric Acids R<sub>2</sub>P(O)ZCH(2)SiMe(3-n)Hal(n)*  
(n=1-3; Z = O, NMe, CH<sub>2</sub>, S)  
Organometallics, (29): 3327-3340 2010.

Dostal, L.; Jambor, R.; Ruzicka, A.; Jirasko, R.; Cernoskova, E.; Benes, L.; de Proft, F.  
*[2+2] Cycloaddition of Carbon Disulfide to NCN-Chelated Organoantimony(III) and Organobismuth(III) Sulfides: Evidence for Terminal Sb-S and Bi-S Bonds in Solution*  
Organometallics, (29): 4486-4490 2010.

Dostal, R.; Londesborough, M. G. S.; Kvicalova, M.; Machacek, J.; Cisarova, I.; Janousek, Z.  
*INCREMENTAL IODINATION OF THE EIGHT-VERTEX closo MONOCARBORANE ANION [closo-1-CB<sub>7</sub>H<sub>8</sub>](-): PREPARATION AND CHARACTERIZATION OF [closo-1-CB<sub>7</sub>H<sub>5</sub>-6,7,8-I-3](-) AND [closo-1-CB<sub>7</sub>H<sub>2</sub>-2,3,4,6,7,8-I-6](-), AND THE SYNTHESIS OF THE FIRST EIGHT-VERTEX C-METHYLATED CARBORANE ANION [1-CH<sub>3</sub>-closo-1-CB<sub>7</sub>H<sub>4</sub>-6,7,8-I-3](-)*  
Collection of Czechoslovak Chemical Communications, (75): 931-947 2010.

Du, J.; Sun, X.; Chen, J.; Jiang, G.  
*The changes in the geometrical, electronic and magnetic properties of titanium clusters as one titanium atom is substituted by boron*  
Journal of Physics B-Atomic Molecular and Optical Physics, (43) 2010.

Duarte, F.; Toro-Labbe, A.  
*The catalytic effect of water on the keto-enol tautomerisation reaction of thioformic acid*  
Molecular Physics, (108): 1375-1384 2010.

Dubis, A. T.; Domagala, M.; Grabowski, S. J.  
*Spectroscopic and theoretical studies on some new pyrrol-2-yl-chloromethyl ketones*  
New Journal of Chemistry, (34): 556-566 2010.

Dudev, T.; Lim, C.  
*Factors Governing the Na<sup>+</sup> vs K<sup>+</sup> Selectivity in Sodium Ion Channels*  
Journal of the American Chemical Society, (132): 2321-2332 2010.

Durka, K.; Kaminski, R.; Lulinski, S.; Serwatowski, J.; Wozniak, K.  
*On the nature of the B center dot center dot center dot N interaction and the conformational flexibility of arylboronic azaesters*  
Physical Chemistry Chemical Physics, (12): 13126-13136 2010.

- Dwivedi, S. D.; Dubey, S. K.; Singh, A. K.; Pandey, K. K.; Pandey, D. S.  
*New ruthenium(II) thiolato complexes: Synthesis, reactivity, spectral, structural and DFT studies*  
Inorganica Chimica Acta, (363): 2095-2103 2010.
- Dyer, H. E.; Huijser, S.; Susperregui, N.; Bonnet, F.; Schwarz, A. D.; Duchateau, R.; Maron, L.; Mountford, P.  
*Ring-Opening Polymerization of rac-Lactide by Bis(phenolate)amine-Supported Samarium Borohydride Complexes: An Experimental and DFT Study*  
Organometallics, (29): 3602-3621 2010.
- Ebrahimi, A.; Habibi-Khorassani, M.; Doosti, M.  
*F-H center dot center dot center dot N hydrogen bonds: Influence of substituent and hybridization of nitrogen on H-bond properties and two-bond F-19-N-15 spin-spin coupling constants ( $(2h)J(F-N)$ )*  
Chemical Physics Letters, (491): 11-16 2010.
- Ebrahimi, A.; Khorassani, S. M. H.; Neyband, R. S.  
*The O center dot center dot center dot H Intramolecular Hydrogen Bond in 4-X-2-Hydroxybenzaldehydes: The Relationships Between Geometrical Parameters, Estimated Binding Energies, and NMR Data*  
International Journal of Quantum Chemistry, (110): 1871-1879 2010.
- Ebrahimi, A.; Khorassani, M. H.; Masoodi, H. R.  
*The role of cation-pi interactions in ethylenic complexes: A theoretical NMR study*  
Chemical Physics Letters, (493): 27-32 2010.
- Ebrahimi, A.; Khorassani, S. M. H.; Delarami, H.; Esmaeeli, H.  
*The effect of CH<sub>3</sub>, F and NO<sub>2</sub> substituents on the individual hydrogen bond energies in the adenine-thymine and guanine-cytosine base pairs*  
Journal of Computer-Aided Molecular Design, (24): 409-416 2010.
- Efremenko, I.; Poverenov, E.; Martin, J. M. L.; Milstein, D.  
*DFT Study of the Structure and Reactivity of the Terminal Pt(IV)-Oxo Complex Bearing No Electron-Withdrawing Ligands*  
Journal of the American Chemical Society, (132): 14886-14900 2010.
- Eisenberg, D.; Jackson, E. A.; Quimby, J. M.; Scott, L. T.; Shenhar, R.  
*The Bicorannulenyl Dianion: A Charged Overcrowded Ethylene*  
Angewandte Chemie-International Edition, (49): 7538-7542 2010.
- El Moncef, A.; El Hadrami, E. M.; Gonzalez, M. A.; Zaballos, E.; Zaragoza, R. J.  
*Experimental and DFT study of the conversion of ephedrine derivatives into oxazolidinones. Double S(N)2 mechanism against S(N)1 mechanism*  
Tetrahedron, (66): 5173-5184 2010.
- Elliott, H. S. A.; Lehmann, J. F.; Mercier, H. P. A.; Jenkins, H. D. B.; Schrobilgen, G. J.

*X-ray Crystal Structures of [XeF][MF<sub>6</sub>] (M = As, Sb, Bi), [XeF][M<sub>2</sub>F<sub>11</sub> (M = Sb, Bi) and Estimated Thermochemical Data and Predicted Stabilities for Noble-Gas Fluorocation Salts using Volume-Based Thermodynamics*  
Inorganic Chemistry, (49): 8504-8523 2010.

Epping, J. D.; Yao, S.; Karni, M.; Apeloig, Y.; Driess, M.  
*Si=X Multiple Bonding with Four-Coordinate Silicon? Insights into the Nature of the Si=O and Si=S Double Bonds in Stable Silanoic Esters and Related Thioesters: A Combined NMR Spectroscopic and Computational Study*  
Journal of the American Chemical Society, (132): 5443-5455 2010.

Erdogdu, Y.; Unsalan, O.; Amalanathan, M.; Joe, I. H.  
*Infrared and Raman spectra, vibrational assignment, NBO analysis and DFT calculations of 6-aminoflavone*  
Journal of Molecular Structure, (980): 24-30 2010.

Eshtiagh-Hosseini, H.; Housaindokht, M. R.; Chahkandi, M.; Morsali, A.  
*A density functional theory investigation of the bromide oxidation mechanism by a vanadium bromoperoxidase model complex*  
Transition Metal Chemistry, (35): 939-947 2010.

Eshtiagh-Hosseini, H.; Yousefi, Z.; Mirzaei, M.; Chen, Y.-G.; Beyramabadi, S. A.; Shokrollahi, A.; Aghaei, R.  
*A new supramolecular compound of chrome(III): Synthesis, spectroscopic characterization, X-ray crystal structure, DFT, and solution studies*  
Journal of Molecular Structure, (973): 1-8 2010.

Esquivel, R. O.; Flores-Gallegos, N.; Carrera, E.; Soriano-Correa, C.  
*Ab initio Study of Selected PAMAM Dendrimers: von Neumann Entropies Analysis*  
Journal of Nano Research, (9): 1-15 2010.

Esteruelas, M. A.; Fernandez-Alvarez, F. J.; Lopez, A. M.; Mora, M.; Onate, E.  
*Borinium Cations as sigma-B-H Ligands in Osmium Complexes*  
Journal of the American Chemical Society, (132): 5600-- 2010.

Esther Sanchez-Castro, M.; Sanchez-Vazquez, M.  
*Electronic and structural study of [BeH<sub>3</sub>](-) ligands coordinated to alkali-metals*  
Journal of Molecular Structure, (969): 204-207 2010.

Etzenbach-Effers, K.; Berkessel, A.  
*Noncovalent Organocatalysis Based on Hydrogen Bonding: Elucidation of Reaction Paths by Computational Methods*  
Asymmetric Organocatalysis, (291): 1-27 2010.

Evans, D. H.; Gruhn, N. E.; Jin, J.; Li, B.; Lorance, E.; Okumura, N.; Macias-Ruvalcaba, N. A.; Zakai, U. I.; Zhang, S. Z.; Block, E.; Glass, R. S.  
*Electrochemical and Chemical Oxidation of Dithia-, Diselena-, Ditellura-, Selenathia-, and Tellurathiamesocycles and Stability of the Oxidized Species*  
Journal of Organic Chemistry, (75): 1997-2009 2010.

Evans, D. H.; Gruhn, N. E.; Jin, J.; Li, B.; Lorance, E.; Okumura, N.; Macias-Ruvalcaba, N. A.; Zakai, U. I.; Zhang, S.-Z.; Block, E.; Glass, R. S.

*Electrochemical and Chemical Oxidation of Dithia-, Diselena-, Ditellura-, Selenathia-, and Tellurathiamesocycles and Stability of the Oxidized Species*  
Journal of Organic Chemistry, (75): 1997-2009 2010.

Fan, X.; Gu, C.; Chen, G.; Ju, X.

*Theoretical Studies on Energetic Property and Stability of Pyrazine and Pyridine Derivatives*  
Chinese Journal of Chemistry, (28): 2364-2370 2010.

Farmanzadeh, D.; Ashtiani, Z.

*Theoretical study of a conjugated aromatic molecular wire*  
Structural Chemistry, (21): 691-699 2010.

Farras, P.; Vinas, C.; Sillanpaa, R.; Teixidor, F.; Rey, M.

*The nature of the chlorination reaction in [1-C<sub>6</sub>H<sub>5</sub>-1-CB<sub>9</sub>H<sub>9</sub>](-) boron clusters*  
Dalton Transactions, (39): 7684-7691 2010.

Farrer, N. J.; Woods, J. A.; Salassa, L.; Zhao, Y.; Robinson, K. S.; Clarkson, G.; Mackay, F. S.; Sadler, P. J.  
*A Potent Trans-Diimine Platinum Anticancer Complex Photoactivated by Visible Light*  
Angewandte Chemie-International Edition, (49): 8905-8908 2010.

Felpin, F.-X.; Miqueu, K.; Sotiropoulos, J.-M.; Fouquet, E.; Ibarguren, O.; Laudien, J.

*Room-Temperature, Ligand- and Base-Free Heck Reactions of Aryl Diazonium Salts at Low Palladium Loading: Sustainable Preparation of Substituted Stilbene Derivatives*  
Chemistry-a European Journal, (16): 5191-5204 2010.

Ferbinteanu, M.; Cimpoesu, F.

*On the Multiple Facets of Aromaticity: Organic, Inorganic, Organometallic, Coordination and Supramolecular Case Studies*  
Studia Universitatis Babes-Bolyai Chemia, (55): 69-87 2010.

Fernandez, I.; Cossio, F. P.; de Cozar, A.; Lledos, A.; Luis Mascarenas, J.

*Concerted and Stepwise Mechanisms in Metal-Free and Metal-Assisted [4+3] Cycloadditions Involving Allyl Cations*  
Chemistry-a European Journal, (16): 12147-12157 2010.

Fernandez, M. I.; Canle, M.; Garcia, M. V.; Santaballa, J. A.

*A theoretical analysis of the acid-base equilibria of hydroxylamine in aqueous solution*  
Chemical Physics Letters, (490): 159-164 2010.

Ferrando-Soria, J.; Castellano, M.; Yuste, C.; Lloret, F.; Julve, M.; Fabelo, O.; Ruiz-Perez, C.; Stiriba, S.-E.; Ruiz-Garcia, R.; Cano, J.

*Long-distance magnetic coupling in dinuclear copper(II) complexes with oligo-para-phenylenediamine bridging ligands*  
Inorganica Chimica Acta, (363): 1666-1678 2010.

- Ferreira, C. A.; Casanovas, J.; Rodrigues, M. A. S.; Mueller, F.; Armelin, E.; Aleman, C.  
*Transport of Metallic Ions through Polyaniline-Containing Composite Membranes*  
Journal of Chemical and Engineering Data, (55): 4801-4807 2010.
- Ferreiros-Martinez, R.; Platas-Iglesias, C.; de Blas, A.; Esteban-Gomez, D.; Rodriguez-Blas, T.  
*Macrocyclic Receptor Showing Improved Pb-II/Zn-II and Pb-II/Ca-II Selectivities*  
European Journal of Inorganic Chemistry: 2495-2503 2010.
- Filatov, A. S.; Rogachev, A. Y.; Jackson, E. A.; Scott, L. T.; Petrukhina, M. A.  
*Increasing the Curvature of a Bowl-Shaped Polyarene by Fullerene-like eta(2)-Complexation of a Transition Metal at the Interior of the Convex Surface*  
Organometallics, (29): 1231-1237 2010.
- Finze, M.; Sprenger, J. A. P.; Schaack, B. B.  
*Salts of the 1-cyanocarba-closo-dodecaborate anions 1-NC-closo-1-CB<sub>11</sub>X<sub>11</sub> (-) (X = H, F, Cl, Br, I)*  
Dalton Transactions, (39): 2708-2716 2010.
- Fischer, R. C.; Power, P. P.  
*pi-Bonding and the Lone Pair Effect in Multiple Bonds Involving Heavier Main Group Elements: Developments in the New Millennium*  
Chemical Reviews, (110): 3877-3923 2010.
- Fischer, R. C.; Power, P. P.  
*pi-Bonding and the Lone Pair Effect in Multiple Bonds Involving Heavier Main Group Elements: Developments in the New Millennium*  
Chemical Reviews, (110): 3877-3923 2010.
- Fitzsimmons, A.; Mori, H.; Miyoshi, E.; Klobukowski, M.  
*Model Core Potential and All-Electron Studies of Molecules Containing Rare Gas Atoms*  
Journal of Physical Chemistry A, (114): 8786-8792 2010.
- Flener-Lovitt, C.; Woon, D. E.; Dunning, T. H., Jr.; Girolami, G. S.  
*A DFT and ab Initio Benchmarking Study of Metal-Alkane Interactions and the Activation of Carbon-Hydrogen Bonds*  
Journal of Physical Chemistry A, (114): 1843-1851 2010.
- Flores Antognini, A.; Robles, N. L.; Cutin, E. H.; Oberhammer, H.  
*Conformational properties of thiazyldifluoride imidosulfurdifluoride, NSF<sub>2</sub>-N=S(F)<sub>2</sub>, and thiazyldifluoride imidosulfuryldifluoride, NSF<sub>2</sub>-N=S(O)F<sub>2</sub>: Vibrational spectra and quantum chemical calculations*  
Journal of Molecular Structure, (976): 3-10 2010.
- Flores-Morales, P.; Gutierrez-Oliva, S.; Silva, E.; Toro-Labbe, A.  
*The reaction electronic flux: A new descriptor of the electronic activity taking place during a chemical reaction. Application to the characterization of the mechanism of the Schiff's base formation in the Maillard reaction*  
Journal of Molecular Structure-Theochem, (943): 121-126 2010.

Fournier, R.

*Density-functional and global optimization study of copper-tin core-shell clusters*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 1071-1078 2010.

Frenking, G.; Holzmann, N.; Neumueller, B.; Dehnicke, K.

*[BeCl<sub>2</sub>(Ph<sub>2</sub>PCH<sub>2</sub>PPh<sub>2</sub>)(2)] - A Donor-Acceptor Complex of Beryllium with the Ligand Bis(diphenylphosphanyl)methane*  
Zeitschrift fur Anorganische und Allgemeine Chemie, (636): 1772-1775 2010.

Fry, A. J.

*The effect of tetramethylammonium ion on the voltammetric behavior of polycyclic aromatic hydrocarbons: computations explain a long-standing anomaly*  
Physical Chemistry Chemical Physics, (12): 14775-14781 2010.

Fu, Y.; Chen, M.; Qi, J.; Shen, W.

*An investigation on the electronic properties of thiadiazoloquinoxaline-based copolymers and the effect of donor-to-acceptor ratio on their properties*  
Journal of Molecular Structure-Theochem, (957): 94-99 2010.

Fu, Y.; Li, J.; Wang, S.-G.

*Bonding and electronic structures in W@Au(12)AE complexes (AE= NO<sup>+</sup>, CO, BF, CN-, or BO-): analogies among ligands isoelectronic to carbon monoxide*  
Journal of Molecular Modeling, (16): 9-16 2010.

Fujiwara, T.; Mochizuki, Y.; Komeiji, Y.; Okiyama, Y.; Mori, H.; Nakano, T.; Miyoshi, E.

*Fragment molecular orbital-based molecular dynamics (FMO-MD) simulations on hydrated Zn(II) ion*  
Chemical Physics Letters, (490): 41-45 2010.

Fujiwara, T.; Mori, H.; Mochizuki, Y.; Tatewaki, H.; Miyoshi, E.

*Theoretical study of hydration models of trivalent rare-earth ions using model core potentials*  
Journal of Molecular Structure-Theochem, (949): 28-35 2010.

Fuks, L.; Gniazdowska, E.; Sadlej-Sosnowska, N.

*Tricarbonyltechnetium(I) and tricarbonylrhenium(I) complexed with N-methyl-2-pyridinecarboxamide as potential radiopharmaceuticals: a computational study*  
Structural Chemistry, (21): 827-835 2010.

Furukawa, T.; Goto, Y.; Kawazoe, J.; Tokunaga, E.; Nakamura, S.; Yang, Y.; Du, H.; Kakehi, A.; Shiro, M.; Shibata, N.

*2-Fluoro-1,3-benzodithiole-1,1,3,3-tetraoxide: A Reagent for Nucleophilic Monofluoromethylation of Aldehydes*  
Angewandte Chemie-International Edition, (49): 1642-1647 2010.

Furukawa, T.; Goto, Y.; Kawazoe, J.; Tokunaga, E.; Nakamura, S.; Yang, Y. D.; Du, H. G.; Kakehi, A.; Shiro, M.; Shibata, N.

*2-Fluoro-1,3-benzodithiole-1,1,3,3-tetraoxide: A Reagent for Nucleophilic Monofluoromethylation of Aldehydes*

Angewandte Chemie-International Edition, (49): 1642-1647 2010.

Fusaro, M.

*A Simple Formula for Evaluation of the Condensed Fukui's Function in Armchair Molecular Models of Nanotubes*

Journal of Computational and Theoretical Nanoscience, (7): 2393-2400 2010.

Fusaro, M.

*Theoretical and Computational Modeling of Functionalization Energy for Armchair Molecular Models of Nanotubes*

Journal of Computational and Theoretical Nanoscience, (7): 1393-1399 2010.

Fustier, M.; Le Goff, X. F.; Le Floch, P.; Mezailles, N.

*Nucleophilic Scandium Carbene Complexes*

Journal of the American Chemical Society, (132): 13108-13110 2010.

Galabov, B.; Koleva, G.; Schaefer, H. F., III; Schleyer, P. v. R.

*Electrophile Affinity: Quantifying Reactivity for the Bromination of Arenes*

Journal of Organic Chemistry, (75): 2813-2819 2010.

Galvez, J.; Guirado, A.

*A Theoretical Study of Topomerization of Imine Systems: Inversion, Rotation or Mixed Mechanisms?*

Journal of Computational Chemistry, (31): 520-531 2010.

Gamez, J. A.; Corral, I.; Mo, O.; Yanez, M.

*Unexpected Gas-Phase Ion Chemistry Results Unraveled by Computational Chemistry*

Current Organic Chemistry, (14): 1600-1611 2010.

Gao, A.; Li, G.; Chang, Y.; Chen, H.; Li, Q.-s.

*Theoretical studies on the structures and properties of As-doped Si-n (n=1-8) clusters*

Journal of Molecular Structure-Theochem, (961): 88-96 2010.

Gao, H.; Zhang, G.; Meng, L.; Chen, D.

*Chiral discrimination in hydrogen-bonded complexes of 2-fluorooxirane with hydrogen peroxide*

Molecular Physics, (108): 2073-2080 2010.

Gao, Y.

*A new specific mechanism for thioacid/azide amidation: electronic and solvent effects*

Central European Journal of Chemistry, (8): 308-319 2010.

Garbounis, D. N.; Tsipis, A. C.; Tsipis, C. A.

*Structural, Electronic, Bonding, Magnetic, and Optical Properties of Bimetallic [RunAum](0+)/(n plus m <= 3) Clusters*

Journal of Computational Chemistry, (31): 2836-2852 2010.

Garcia, G.; Granadino-Roldan, J. M.; Garzon, A.; Moral, M.; Pena-Ruiz, T.; Navarro, A.; Paz Fernandez-Liencres, M.; Fernandez-Gomez, M.

*Theoretical Study of Bis(phenylethyanyl)thienoacenes as Precursors of Molecular Wires for Molecular Electronics*  
Journal of Physical Chemistry C, (114): 12325-12334 2010.

Garcia, G.; Navarro, A.; Manuel Granadino-Roldan, J.; Garzon, A.; Pena Ruiz, T.; Paz Fernandez-Liencres, M.; Melguizo, M.; Penas, A.; Pongor, G.; Eori, J.; Fernandez-Gomez, M.  
*Molecular structure, conformational preferences and vibrational analysis of 2-hydroxystyrene: A computational and spectroscopic research*  
Chemical Physics, (374): 62-76 2010.

Geng, Z.; Wang, Y.; Wang, Y.; Liang, J.; Sheng, Y.; Sun, X.  
*Theoretical Study on the Reaction Mechanism of n-Butene Anion with N<sub>2</sub>O in Gas Phase*  
Acta Chimica Sinica, (68): 391-402 2010.

Gertych, A.; Koput, J.  
*Ab Initio Prediction of the Structure and Vibration-Rotation Spectroscopic Properties of Na<sub>2</sub>OH and K<sub>2</sub>OH*  
Journal of Computational Chemistry, (31): 1542-1549 2010.

Ghereg, D.; Andre, E.; Sotiropoulos, J.-M.; Miqueu, K.; Gornitzka, H.; Escudie, J.  
*1,3-Dipole Behavior of Phosphagermaallene Tip(tBu)Ge=C=PMes\* Leading to a Phosphagermaheterocyclic Carbene*  
Angewandte Chemie-International Edition, (49): 8704-8707 2010.

Gholivand, K.; Mahzouni, H. R.; Esrafil, M. D.  
*How do phosphoramides compete with phosphine oxides in lanthanide complexation? Structural, electronic and energy aspects at ab initio and DFT levels*  
Theoretical Chemistry Accounts, (127): 539-550 2010.

Giagou, T.; Meyer, M. P.  
*Mechanism of the Swern Oxidation: Significant Deviations from Transition State Theory*  
Journal of Organic Chemistry, (75): 8088-8099 2010.

Girichev, G. V.; Giricheva, N. I.; Golubchikov, O. A.; Mimenkov, Y. V.; Semeikin, A. S.; Shlykov, S. A.  
*Octamethylporphyrin copper, C<sub>28</sub>H<sub>28</sub>N<sub>4</sub>Cu - A first experimental structure determination of porphyrins in gas phase*  
Journal of Molecular Structure, (978): 163-169 2010.

Goekcinar, E.; Karaghiosoff, K.; Klaoetke, T. M.; Evangelisti, C.; Rotter, C.  
*Structure and Bonding in the Trichalcogenometaphosphate-Pyridine Anions [PX<sub>3</sub>-Py]<sup>-</sup> (X = O, S, Se, Te)*  
Phosphorus Sulfur and Silicon and the Related Elements, (185): 2527-2534 2010.

Gonzalez-Castrillo, A.; Hurtado, M.; Mo, O.; Yanez, M.; Guillemin, J.-C.  
*The role of hyperconjugative aromaticity in the enhanced acidity of methyl-, silyl and germylcyclopentadienes*  
Molecular Physics, (108): 2467-2476 2010.

Gourlaouen, C.; Parisel, O.; Piquemal, J. P.  
*Importance of backdonation in [M-(CO)](p+) complexes isoelectronic to [Au-(CO)](+)*  
Journal of Chemical Physics, (133) 2010.

Grabowski, S. J.; Ugalde, J. M.  
*Ab initio calculations on C<sub>6</sub>H<sub>6</sub> center dot center dot center dot(HF)(n) clusters - X-H center dot center dot center dot pi hydrogen bond*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 769-778 2010.

Grabowski, S. J.; Ugalde, J. M.  
*Bond Paths Show Preferable Interactions: Ab Initio and QTAIM Studies on the X-H center dot center dot center dot pi Hydrogen Bond*  
Journal of Physical Chemistry A, (114): 7223-7229 2010.

Grabowski, S. J.; Ugalde, J. M.  
*High-level ab initio calculations on low barrier hydrogen bonds and proton bound homodimers*  
Chemical Physics Letters, (493): 37-44 2010.

Griaznova, T. P.; Katsyuba, S. A.; Shakirova, O. G.; Lavrenova, L. G.  
*Variable temperature IR spectroscopy and quantum chemistry as the tool for diagnostics of metal spin state*  
Chemical Physics Letters, (495): 50-54 2010.

Gu, J.; Wang, J.; Leszczynski, J.  
*Electron attachment-induced DNA single-strand breaks at the pyrimidine sites*  
Nucleic Acids Research, (38): 5280-5290 2010.

Gu, J.; Wong, N.-B.; Xie, Y.; Schaefer, F. H., III  
*Electron Attachment to a Hydrated DNA Duplex: The Dinucleoside Phosphate Deoxyguanylyl-3',5'-Deoxycytidine*  
Chemistry-a European Journal, (16): 13155-13162 2010.

Gu, J.; Xie, Y.; Schaefer, H. F., III  
*Electron Attachment to Hydrated Oligonucleotide Dimers: Guanylyl-3',5'-Cytidine and Cytidylyl-3',5'-Guanosine*  
Chemistry-a European Journal, (16): 5089-5096 2010.

Gualco, P.; Mercy, M.; Ladeira, S.; Coppel, Y.; Maron, L.; Amgoune, A.; Bourissou, D.  
*Hypervalent Silicon Compounds by Coordination of Diphosphine-Silanes to Gold*  
Chemistry-a European Journal, (16): 10808-10817 2010.

Guermoune, A.; Cherqaoui, D.; Jarid, A.; Liebman, J. F.  
*Structure and decomposition of [HFe(CO)(4)(B<sub>2</sub>H<sub>5</sub>)], a revised behavior of an old uncharacterized complex*  
Journal of Organometallic Chemistry, (695): 1715-1721 2010.

Guha, A. K.; Phukan, A. K.

*Theoretical study on the mechanism of catalytic reduction of hydrazine to ammonia mediated by vanadium (III) thiolate complexes*  
Inorganica Chimica Acta, (363): 3270-3273 2010.

Guha, A. K.; Sarmah, S.; Phukan, A. K.  
*Effect of substituents at the heteroatom on the structure and ligating properties of heterocyclic carbene, silylene, germylene and abnormal carbene: A theoretical study*  
Dalton Transactions, (39): 7374-7383 2010.

Guillon, T.; Boggio-Pasqua, M.; Alary, F.; Heully, J.-L.; Lebon, E.; Sutra, P.; Igau, A.  
*Theoretical Investigation on the Photophysical Properties of Model Ruthenium Complexes with Diazabutadiene Ligands [Ru(bpy)(3-x)(dab)(x)](2+) (x=1-3)*  
Inorganic Chemistry, (49): 8862-8872 2010.

Guin, M.; Maity, S.; Patwari, G. N.  
*Infrared-Optical Double Resonance Spectroscopic Measurements on 2-(2'-Pyridyl)benzimidazole and its Hydrogen Bonded Complexes with Water and Methanol*  
Journal of Physical Chemistry A, (114): 8323-8330 2010.

Guo, J.; Lau, K.-C.; Xi, H.-W.; Lim, K. H.; So, C.-W.  
*Synthesis and characterization of a tin(II) bis(phosphinoyl)methanediide complex: a stannavinylidene derivative*  
Chemical Communications, (46): 1929-1931 2010.

Guo, J.; Zhang, D.; Duan, C.; Liu, C.  
*Probing anion-cellulose interactions in imidazolium-based room temperature ionic liquids: a density functional study*  
Carbohydrate Research, (345): 2201-2205 2010.

Guo, J.; Zhang, D.; Liu, C.  
*A Theoretical Investigation of the Interactions between Cellulose and 1-Butyl-3-Methylimidazolium Chloride*  
Journal of Theoretical & Computational Chemistry, (9): 611-624 2010.

Guo, J.-C.  
*[M(C<sub>6</sub>Li<sub>6</sub>)(2)](n-) (M = Nb, Ta, Mo and W; n=1, 0): Sandwich complexes containing star-like hexolithiobenzenes*  
Journal of Molecular Structure-Theochem, (953): 139-142 2010.

Guo, J. C.; Li, J. G.  
*C<sub>5</sub>Li<sub>5</sub> Zn-n C<sub>5</sub>Li<sub>5</sub> (n=2-8): Novel sandwich complexes containing -Zn-Zn- chain*  
Journal of Molecular Structure-Theochem, (942): 43-46 2010.

Guo, J.-C.; Li, J.-G.  
*[C<sub>5</sub>Li<sub>5</sub>]Zn-n[C<sub>5</sub>Li<sub>5</sub>] (n=2-8): Novel sandwich complexes containing -Zn-Zn- chain*  
Journal of Molecular Structure-Theochem, (942): 43-46 2010.

Guo, J. Y.; Lau, K. C.; Xi, H. W.; Lim, K. H.; So, C. W.

*Synthesis and characterization of a tin(II) bis(phosphinoyl)methanediide complex: a stannavinylidene derivative*  
Chemical Communications, (46): 1929-1931 2010.

Guo, Y.; Tao, G.-H.; Blumenfeld, A.; Shreeve, J. n. M.  
*Impact of Silyl Enol Ether Stability on Palladium-Catalyzed Arylations*  
Organometallics, (29): 1818-1823 2010.

Gushehin, P. V.; Starova, G. L.; Haukka, M.; Kuznetsov, M. L.; Eremenko, I. L.; Kukushkin, V. Y.  
*Chloride-Chloroform Clusters Exhibiting Weak Hydrogen and Halogen Bondings Are Fully Characterized in the Solid State by X-ray Diffraction*  
Crystal Growth & Design, (10): 4839-4846 2010.

Gutsev, G. L.; Weatherford, C. A.; Pradhan, K.; Jena, P.  
*Structure and Spectroscopic Properties of Iron Oxides with the High Content of Oxygen: FeOn and FeOn- (n=5-12)*  
Journal of Physical Chemistry A, (114): 9014-9021 2010.

Gyepes, R.; Varga, V.; Horacek, M.; Kubista, J.; Pinkas, J.; Mach, K.  
*Influence of the Ti-O-C Angle on the Oxygen-to-Titanium pi-Donation in [Cp-2\*Ti(III)OR] Complexes*  
Organometallics, (29): 3780-3789 2010.

Haghdadi, M.; Price, L. S.; Bosra, H. G.  
*Analysis of anomeric effects in some oxa diaza Spiro decan derivatives by DFT molecular orbital calculations*  
Journal of Molecular Structure-Theochem, (947): 58-67 2010.

Hahn, J. R.; Kang, H. S.  
*Role of molecular orientation in vibration, hopping, and electronic properties of single pyridine molecules adsorbed on Ag(110) surface: A combined STM and DFT study*  
Surface Science, (604): 258-264 2010.

Halling, M. D.; Bell, J. D.; Pugmire, R. J.; Grant, D. M.; Miller, J. S.  
*Solid-State NMR Spectra and Long, Intra-Dimer Bonding in the pi-[TTF](2)(2+) (TTF = Tetrathiafulvalene) Dication*  
Journal of Physical Chemistry A, (114): 6622-6629 2010.

Han, S.; Yoo, H. S.; Kim, S. K.  
*Conformer-Specific Ionization Spectroscopy of Bromocyclohexane: Equatorial versus Axial Conformers*  
Journal of Physical Chemistry A, (114): 10005-10010 2010.

Handzlik, J.  
*Computational study of the properties and metathesis activity of Mo methylidene species in HZSM-5 zeolite*  
Journal of Molecular Catalysis a-Chemical, (316): 106-111 2010.

Harb, M.; Rabilloud, F.; Simon, D.  
*Structural, electronic, magnetic and optical properties of icosahedral silver-nickel nanoclusters*  
Physical Chemistry Chemical Physics, (12): 4246-4254 2010.

Hasegawa, M.; Usui, I.; Konno, S.; Murakami, M.  
*Substituent effect of group 14 elements on the ring-opening reaction of cyclobutene*  
Organic & Biomolecular Chemistry, (8): 4169-4175 2010.

He, H.; Zapol, P.; Curtiss, L. A.  
*A Theoretical Study of CO<sub>2</sub> Anions on Anatase (101) Surface*  
Journal of Physical Chemistry C, (114): 21474-21481 2010.

He, Q.; Huo, A.-X.; Meng, X.-J.; Yang, J.  
*Theoretical Study on Hydrogen Interaction between 5-Fluorouracil and Glycine*  
Chinese Journal of Structural Chemistry, (29): 738-746 2010.

He, S.; Tan, Y.; Xiao, X.; Zhu, L.; Guo, Y.; Li, M.; Tian, A.; Pu, X.; Wong, N.-B.  
*Substituent effects on electronic character of the C=N group and trans/cis isomerization in the C-substituted imine derivatives: A computational study*  
Journal of Molecular Structure-Theochem, (951): 7-13 2010.

He, Y.; Xue, Y.  
*Mechanism Insight into the Cyanide-Catalyzed Benzoin Condensation: A Density Functional Theory Study*  
Journal of Physical Chemistry A, (114): 9222-9230 2010.

He, Z.-W.; Zhou, S.-Q.; Ju, X.-H.; Liu, Z.-L.  
*Computational investigation on 2,6-diamino-3,5-dinitropyridine-1-oxide crystal*  
Structural Chemistry, (21): 651-656 2010.

Hemelsoet, K.; Van Durme, F.; Van Speybroeck, V.; Reyniers, M. F.; Waroquier, M.  
*Bond Dissociation Energies of Organophosphorus Compounds: an Assessment of Contemporary Ab Initio Procedures*  
Journal of Physical Chemistry A, (114): 2864-2873 2010.

Hemelsoet, K.; Van Durme, F.; Van Speybroeck, V.; Reyniers, M.-F.; Waroquier, M.  
*Bond Dissociation Energies of Organophosphorus Compounds: an Assessment of Contemporary Ab Initio Procedures*  
Journal of Physical Chemistry A, (114): 2864-2873 2010.

Hernandez-Altamirano, R.; Mena-Cervantes, V. Y.; Perez-Miranda, S.; Fernandez, F. J.; Andres Flores-Sandoval, C.; Barba, V.; Beltran, H. I.; Zamudio-Rivera, L. S.  
*Molecular design and QSAR study of low acute toxicity biocides with 4,4'-dimorpholyl-methane core obtained by microwave-assisted synthesis*  
Green Chemistry, (12): 1036-1048 2010.

Hernandez-Rivera, S. P.; Infante-Castillo, R.

*A systematic theoretical investigation of the relationship between heats of detonation and NBO charges and N-15 NMR chemical shifts of nitro groups in nitramines and nitro paraffins*  
Journal of Molecular Structure-Theochem, (960): 57-62 2010.

Hernandez-Rojas, J.; Calvo, F.; Rabilloud, F.; Breton, J.; Gomez Llorente, J. M.  
*Modeling Water Clusters on Cationic Carbonaceous Seeds*  
Journal of Physical Chemistry A, (114): 7267-7274 2010.

Heyl, D. L.; Osborne, J. M.; Pamarthi, S.; Samisetti, S.; Gray, A. W.; Jayaprakash, A.; Konda, S.; Brown, D. J.; Miller, S. R.; Eizadkhah, R.; Milletti, M. C.  
*Liposome Damage and Modeling of Fragments of Human Islet Amyloid Polypeptide (IAPP) Support a Two-Step Model of Membrane Destruction*  
International Journal of Peptide Research and Therapeutics, (16): 43-54 2010.

Hildebrand, A.; Sarosi, M. B.; Loennecke, P.; Silaghi-Dumitrescu, L.; Hey-Hawkins, E.  
*UNSYMMETRICAL DINUCLEAR RHODIUM COMPLEXES WITH ARSANYL- AND PHOSPHANYLARYLTHIOLATO LIGANDS [Rh(mu-S-2-EPh<sub>2</sub>C<sub>6</sub>H<sub>4</sub>-kappa S-2,E)(2)Rh(cod)] (E = As, P)*  
Revue Roumaine de Chimie, (55): 885-+ 2010.

Hilder, T. A.; Yang, R.; Ganesh, V.; Gordon, D.; Bliznyuk, A.; Rendell, A. P.; Chung, S. H.  
*Validity of current force fields for simulations on boron nitride nanotubes*  
Micro & Nano Letters, (5): 150-156 2010.

Hnyk, D.; Holub, J.; Jelinek, T.; Machacek, J.; Londesborough, M. G. S.  
*Revisiting B<sub>20</sub>h<sub>16</sub> by Means of a Joint Computational/Experimental NMR Approach*  
Collection of Czechoslovak Chemical Communications, (75): 1115-1123 2010.

Hnyk, D.; Vsetecka, V.; Droz, L.  
*Charge distribution within hypercarbon-halogenated 1-Ph-2-X-1,2-dicarba-closo-dodecaboranes, (X = F, Cl, Br, I): A dipole moment and computational study*  
Journal of Molecular Structure, (978): 246-249 2010.

Ho, C.-H.; Chu, Y.-Y.; Lin, C.-N.; Chen, H.-W.; Huang, C.-Y.; Shieh, M.  
*Selenium-Manganese Carbonyl Clusters: Synthesis, Reversible Transformation, Electrochemical Properties, and Theoretical Calculations*  
Organometallics, (29): 4396-4405 2010.

Hodgson, J. L.; Coote, M. L.  
*Clarifying the Mechanism of the Denisov Cycle: How do Hindered Amine Light Stabilizers Protect Polymer Coatings from Photo-oxidative Degradation?*  
Macromolecules, (43): 4573-4583 2010.

Hollo, B.; Leovac, V. M.; Bombicz, P.; Kovacs, A.; Jovanovic, L. S.; Bogdanovic, G.; Kojic, V.; Divjakovic, V.; Joksovic, M. D.; Szecsenyi, K. M.  
*Synthesis, Structural, DFT, and Cytotoxicity Studies of Cu-II and Ni-II Complexes with 3-Aminopyrazole Derivatives*  
Australian Journal of Chemistry, (63): 1557-1564 2010.

- Holt, A.; Bostrom, J.; Karlstrom, G.; Lindh, R.  
*A NEMO Potential that Includes the Dipole-Quadrupole and Quadrupole-Quadrupole Polarizability*  
Journal of Computational Chemistry, (31): 1583-1591 2010.
- Hong, J.; Lee, C.; Ham, S.  
*Molecular Dynamics Simulation and Density Functional Theory Investigation for Thiacalix 4 biscrown and its Complexes with Alkali-Metal Cations*  
Bulletin of the Korean Chemical Society, (31): 453-456 2010.
- Hooper, J.; Sauer, E. L. O.; Arns, S.; Woo, T. K.; Barriault, L.  
*On the Origin of Altered Diastereomeric Ratios for Anionic versus Neutral Reaction Conditions in the Oxy-Cope/Ene Reaction: An Interplay of Experiment and Computational Modeling*  
Chemistry-a European Journal, (16): 14124-14130 2010.
- Horacek, M.; Gyepes, R.; Merna, J.; Kubista, J.; Mach, K.; Pinkas, J.  
*Dinuclear titanium complexes with methylphenylsilylene bridge between cyclopentadienyl rings. Synthesis, characterization and reactivity towards ethylene*  
Journal of Organometallic Chemistry, (695): 1425-1433 2010.
- Horvath, S.; McCoy, A. B.; Elliott, B. M.; Weddle, G. H.; Roscioli, J. R.; Johnson, M. A.  
*Anharmonicities and Isotopic Effects in the Vibrational Spectra of X-center dot H<sub>2</sub>O, center dot HDO, and center dot D<sub>2</sub>O [X = Cl, Br, and I] Binary Complexes*  
Journal of Physical Chemistry A, (114): 1556-1568 2010.
- Houriez, C.; Masella, M.; Ferre, N.  
*Structural and atoms-in-molecules analysis of hydrogen-bond network around nitroxides in liquid waters*  
Journal of Chemical Physics, (133) 2010.
- Howard, A. A.; Tschumper, G. S.; Hammer, N. I.  
*Effects of Hydrogen Bonding on Vibrational Normal Modes of Pyrimidine*  
Journal of Physical Chemistry A, (114): 6803-6810 2010.
- Hrobarik, P.; Sigmundova, I.; Zahradnik, P.; Kasak, P.; Arion, V.; Franz, E.; Clays, K.  
*Molecular Engineering of Benzothiazolium Salts with Large Quadratic Hyperpolarizabilities: Can Auxiliary Electron-Withdrawing Groups Enhance Nonlinear Optical Responses?*  
Journal of Physical Chemistry C, (114): 22289-22302 2010.
- Hrobarikova, V.; Hrobarik, P.; Gajdos, P.; Fitis, I.; Fakis, M.; Persephonis, P.; Zahradnik, P.  
*Benzothiazole-Based Fluorophores of Donor-pi-Acceptor-pi-Donor Type Displaying High Two-Photon Absorption*  
Journal of Organic Chemistry, (75): 3053-3068 2010.
- Hu, F.; Zhang, Y.; Zhang, H.; Li, L.; Tian, A.  
*Density Functional Theory Study on Hydrogen Bonding Interaction of Catechin-(H<sub>2</sub>O)(n)*  
Chinese Journal of Chemistry, (28): 741-747 2010.

Hu, Y.; Ma, H.-X.; Li, J.-F.; Gao, R.; Song, J.-R.  
*Density Functional Theoretical Study on Intermolecular Interactions of 3,6-Dihydrazino-1,2,4,5-tetrazine Dimers*  
Bulletin of the Korean Chemical Society, (31): 2897-2902 2010.

Hu, Y.-Y.; Sun, S.-L.; Muhammad, S.; Xu, H.-L.; Su, Z.-M.  
*How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene*  
Journal of Physical Chemistry C, (114): 19792-19798 2010.

Hua, S.; Hua, W.; Li, S.  
*An Efficient Implementation of the Generalized Energy-Based Fragmentation Approach for General Large Molecules*  
Journal of Physical Chemistry A, (114): 8126-8134 2010.

Huang, F.; Lu, G.; Zhao, L.; Li, H.; Wang, Z.-X.  
*The Catalytic Role of N-Heterocyclic Carbene in a Metal-Free Conversion of Carbon Dioxide into Methanol: A Computational Mechanism Study*  
Journal of the American Chemical Society, (132): 12388-12396 2010.

Huang, H.; Rheingold, A. L.; Hughes, R. P.  
*Synthesis and X-ray Structure of a Diamagnetic Oxo-Bridged Trifluoromethyl-Chromium(V) Complex: Structural and Computational Comparisons between CF<sub>3</sub> and CH<sub>3</sub> Ligands in Two Different Oxidation States of Chromium*  
Organometallics, (29): 3672-3675 2010.

Huang, H.; Zhang, T.; Zhang, J.; Wang, L.  
*A screened hybrid density functional study on energetic complexes: Cobalt, nickel and copper carbohydrazide perchlorates*  
Journal of Hazardous materials, (179): 21-27 2010.

Huang, H.; Zhang, T.; Zhang, J.; Wang, L.; Yang, L.; Qiao, X.; Shang, J.  
*Theoretical Studies on the Structures and Properties of Energetic Complexes: Cobalt, Nickel and Copper Carbohydrazide Nitrates*  
Acta Chimica Sinica, (68): 289-293 2010.

Huang, H. S.; Zhang, T. L.; Zhang, J. G.; Wang, L. Q.; Yang, L.; Qiao, X. J.; Shang, J.  
*Theoretical Studies on the Structures and Properties of Energetic Complexes: Cobalt, Nickel and Copper Carbohydrazide Nitrates*  
Acta Chimica Sinica, (68): 289-293 2010.

Huang, W.; Llano, J.; Gauld, J. W.  
*Redox Mechanism of Glycosidic Bond Hydrolysis Catalyzed by 6-Phospho-alpha-glucosidase: A DFT Study*  
Journal of Physical Chemistry B, (114): 11196-11206 2010.

Huang, Z.; Dai, Y.; Yu, L.  
*Density functional theory and topological analysis on the hydrogen bonding interactions in N-protonated adrenaline-DMSO complexes*

Structural Chemistry, (21): 863-872 2010.

Huang, Z.; Yu, L.; Dai, Y.

*Combined DFT with NBO and QTAIM studies on the hydrogen bonds in (CH<sub>3</sub>OH) (n) (n=2-8) clusters*

Structural Chemistry, (21): 565-572 2010.

Huang, Z.; Yu, L.; Dai, Y.

*Density functional theory and topological analysis on the hydrogen bonds in cysteine-propanoic acid complexes*

Structural Chemistry, (21): 855-862 2010.

Huang, Z.; Yu, L.; Dai, Y.; Wang, H.

*Hydrogen bonding interactions in cysteine-urea complexes: Theoretical studies of structures, properties and topologies*

Journal of Molecular Structure-Theochem, (960): 98-105 2010.

Hughes, M. J.; Gerken, M.; Mercier, H. P. A.; Schrobilgen, G. J.

*Syntheses and Multi-NMR Study of fac- and mer-OsO<sub>3</sub>F<sub>2</sub>(NCCH<sub>3</sub>) and the X-ray Crystal Structure (n=2) and Raman Spectrum (n=0) of fac-OsO<sub>3</sub>F<sub>2</sub>(NCCH<sub>3</sub>)center dot nCH(3)CN*

Inorganic Chemistry, (49): 4768-4780 2010.

Hughes, M. J.; Mercier, H. P. A.; Schrobilgen, G. J.

*Fluoride Ion Donor Properties of cis-OsO<sub>2</sub>F<sub>4</sub>: Synthesis, Raman Spectroscopic Study, and X-ray Crystal Structure of [OsO<sub>2</sub>F<sub>3</sub>][Sb<sub>2</sub>F<sub>11</sub>]*

Inorganic Chemistry, (49): 271-284 2010.

Hughes, M. J.; Mercier, H. P. A.; Schrobilgen, G. J.

*Syntheses, Raman Spectra, and X-ray Crystal Structures of [XeF<sub>5</sub>][μ-F(OsO<sub>3</sub>F<sub>2</sub>)(2)] and [M][OsO<sub>3</sub>F<sub>3</sub>] (M = XeF<sub>5</sub><sup>+</sup>, Xe<sub>2</sub>F<sub>11</sub><sup>+</sup>)*

Inorganic Chemistry, (49): 3501-3515 2010.

Hull, J. F.; Balcells, D.; Sauer, E. L. O.; Raynaud, C.; Brudvig, G. W.; Crabtree, R. H.; Eisenstein, O.

*Manganese Catalysts for C-H Activation: An Experimental/Theoretical Study Identifies the Stereoelectronic Factor That Controls the Switch between Hydroxylation and Desaturation Pathways*

Journal of the American Chemical Society, (132): 7605-7616 2010.

Hurtado, M.; Lamsabhi, A.-M.; Mo, O.; Yanez, M.; Guillemin, J.-C.

*Are cyclopentadienylberyllium, magnesium and calcium hydrides carbon or metal acids in the gas phase?*

Dalton Transactions, (39): 4593-4601 2010.

Ignatyev, I. S.; Montejo, M.; Lopez Gonzalez, J. J.

*Theoretical study of the mechanisms of the hydrolysis and condensation reactions of silicon and titanium alkoxides: similarities and differences*

Dalton Transactions, (39): 6967-6973 2010.

Iker, D. R.; Iann C, G.; Romuald, P.; Laurent, M.  
*Grafting of Lanthanide Complexes on Silica Surfaces: A Theoretical Investigation*  
Journal of Physical Chemistry A, (114): 6322-6330 2010.

Ikezawa, Y.; Nagai, A.  
*IR and UV-visible spectroscopic studies of the adsorption of 3-fluorobenzoic acid on Au(111), Au(100) and Au(110) electrodes in neutral solution*  
Electrochimica Acta, (55): 8901-8907 2010.

Ilichev, V. A.; Katkova, M. A.; Ketkov, S. Y.; Isachenkov, N. A.; Konev, A. N.; Fukin, G. K.; Bochkarev, M. N.  
*Scandium 2-mercaptopbenzothiazolate: Synthesis, structure and electroluminescent properties*  
Polyhedron, (29): 400-404 2010.

Iriarte, A. G.; Arguello, G. A.  
*Study of the influence of stereoelectronic interactions on the vibrational frequencies of a series of peroxy fluorocarboxygenated compounds*  
Journal of Molecular Structure, (978): 20-25 2010.

Irshaidat, T.  
*A DFT Study on Selected Physical Organic Aspects of the Fischer Carbene Intermediates [(M(CO)(4)(C(OMe)Me)]*  
E-Journal of Chemistry, (7): 437-444 2010.

Irshaidat, T.  
*What can the geometry tell about the charge distribution in the mesoionic heterocycles? A DFT study on the SCN<sub>4</sub>R<sub>2</sub> system*  
Journal of Physical Organic Chemistry, (23): 67-74 2010.

Isabel Ortiz, M.; Laura Soriano, M.; Pilar Carranza, M.; Jalon, F. A.; Steed, J. W.; Mereiter, K.; Rodriguez, A. M.; Quinonero, D.; Deya, P. M.; Manzano, B. R.  
*New [2 x 2] Copper(I) Grids as Anion Receptors. Effect of Ligand Functionalization on the Ability to Host Counteranions by Hydrogen Bonds*  
Inorganic Chemistry, (49): 8828-8847 2010.

Ishikawa, A.; Nakao, Y.; Sato, H.; Sakaki, S.  
*Pd(II)-promoted direct cross-coupling reaction of arenes via highly regioselective aromatic C-H activation: a theoretical study*  
Dalton Transactions, (39): 3279-3289 2010.

Ishikawa, S.; Yamabe, T.  
*A theoretical study of hydrogen adsorption on Li, Be, Na, and Mg atoms attached to aromatic hydrocarbons*  
Applied Physics a-Materials Science & Processing, (99): 29-37 2010.

Ivanistsev, V.; Nazmutdinov, R. R.; Lust, E.  
*Density functional theory study of the water adsorption at Bi(111) electrode surface*  
Surface Science, (604): 1919-1927 2010.

- Ivashin, N. V.  
*IR spectrum and localization of excitation of reaction center of photosystem II in triplet state*  
Optics and Spectroscopy, (108): 598-607 2010.
- Iwano, K.; Shimoji, Y.  
*Strong Electron Correlation in the High-Temperature Phase of (EDO-TTF)(2)PF<sub>6</sub> as a Quasi-One-Dimensional Molecular Conductor*  
Journal of the Physical Society of Japan, (79) 2010.
- Izgorodina, E. I.; Chesman, A. S. R.; Turner, D. R.; Deacon, G. B.; Batten, S. R.  
*Theoretical and Experimental Insights into the Mechanism of the Nucleophilic Addition of Water and Methanol to Dicyanonitrosomethanide*  
Journal of Physical Chemistry B, (114): 16517-16527 2010.
- Jakobsche, C. E.; Choudhary, A.; Miller, S. J.; Raines, R. T.  
*n -> pi\*(star) Interaction and n(pi) Pauli Repulsion Are Antagonistic for Protein Stability*  
Journal of the American Chemical Society, (132): 6651-+ 2010.
- Janicki, R.; Starynowicz, P.  
*Charge density distribution in aminomethylphosphonic acid*  
Acta Crystallographica Section B-Structural Science, (66): 559-567 2010.
- Jeanvoine, Y.; Spezia, R.  
*Cu<sup>2+</sup> binding chalcogen-chalcogen bridges: A problematic case for DFT*  
Journal of Molecular Structure-Theochem, (954): 7-15 2010.
- Jensen, F.  
*Describing Anions by Density Functional Theory: Fractional Electron Affinity*  
Journal of Chemical Theory and Computation, (6): 2726-2735 2010.
- Jenter, J.; Roesky, P. W.; Ajellal, N.; Guillaume, S. M.; Susperregui, N.; Maron, L.  
*Bis(phosphinimino)methanide Borohydride Complexes of the Rare-Earth Elements as Initiators for the Ring-Opening Polymerization of epsilon-Caprolactone: Combined Experimental and Computational Investigations*  
Chemistry-a European Journal, (16): 4629-4638 2010.
- Jian, F.; Wang, J.; Xiao, H.; Zhao, P.; Sun, P.; Huang, L.  
*[60]Fullerene metal complexes with large effective two-photon absorption cross-section*  
Dalton Transactions, (39): 11045-11052 2010.
- Jiang, X.; Wang, C.  
*Evaluation of the individual hydrogen bonding energies in N-methylacetamide chains*  
Science China-Chemistry, (53): 1754-1761 2010.
- Jiang, Z.; Yang, H.; Han, X.; Luo, J.; Wong, M. W.; Lu, Y.  
*Direct asymmetric aldol reactions between aldehydes and ketones catalyzed by L-tryptophan in the presence of water*  
Organic & Biomolecular Chemistry, (8): 1368-1377 2010.

- Jiang, Z. Q.; Yang, H.; Han, X.; Luo, J.; Wong, M. W.; Lu, Y. X.  
*Direct asymmetric aldol reactions between aldehydes and ketones catalyzed by L-tryptophan in the presence of water*  
Organic & Biomolecular Chemistry, (8): 1368-1377 2010.
- Jiao, Y.-Q.; Lu, G.-W.; Zhao, K.; Chen, Y.; Lan, J.-H.; Shao, C.-J.; Wang, A.-J.; Zhang, P.; Zhang, W.-S.; Zhou, G.-G.; Yang, Z.-Q.; Wang, M.  
*Theoretical studies on metal-metal interaction and luminescence of a dinuclear [AuS<sub>2</sub>PH<sub>2</sub>](2) complex*  
Journal of Molecular Structure-Theochem, (957): 1-5 2010.
- Jimenez-Halla, J. O. C.; Wu, Y.-B.; Wang, Z.-X.; Islas, R.; Heine, T.; Merino, G.  
*CAI4Be and CAI3Be2-: global minima with a planar pentacoordinate carbon atom*  
Chemical Communications, (46): 8776-8778 2010.
- Jin, L.; Wu, Y.; Kim, C. K.; Xue, Y.  
*Theoretical study on the aminolysis of ester catalyzed by TBD: Hydrogen bonding or covalent bonding of the catalyst?*  
Journal of Molecular Structure-Theochem, (942): 137-144 2010.
- Jin, L.; Wu, Y.; Kim, C.-k.; Xue, Y.  
*Theoretical study on the aminolysis of ester catalyzed by TBD: Hydrogen bonding or covalent bonding of the catalyst?*  
Journal of Molecular Structure-Theochem, (942): 137-144 2010.
- Jin, P.; Li, F.; Riley, K.; Lenoir, D.; Schleyer, P. V. R.; Chen, Z.  
*What Is the Preferred Structure of the Meisenheimer-Wheland Complex Between sym-Triaminobenzene and 4,6-Dinitrobenzofuran?*  
Journal of Organic Chemistry, (75): 3761-3765 2010.
- Jing, B.; Li, Q.; Gong, B.; Cheng, J.; Li, W.; Liu, Z.  
*A theoretical analysis of the weakly bound complexes HM center dot center dot center dot HXY (M=O and S; XY=CN and NC): comparison with H<sub>2</sub>M center dot center dot center dot HXY complexes*  
Molecular Physics, (108): 1655-1664 2010.
- Jo, E.; Jhon, Y. H.; Choi, S. B.; Shim, J.-G.; Kim, J.-H.; Lee, J. H.; Lee, I.-Y.; Jang, K.-R.; Kim, J.  
*Crystal structure and electronic properties of 2-amino-2-methyl-1-propanol (AMP) carbamate*  
Chemical Communications, (46): 9158-9160 2010.
- Johansson, C.; Lloyd-Jones, G. C.; Norrby, P.-O.  
*Memory and dynamics in Pd-catalyzed allylic alkylation with P,N-ligands*  
Tetrahedron-Asymmetry, (21): 1585-1592 2010.
- John, A.; Shaikh, M. M.; Butcher, R. J.; Ghosh, P.  
*Highly efficient palladium precatalysts of homoscorpionate bispyrazolyl ligands for the more challenging Suzuki-Miyaura cross-coupling of aryl chlorides*

Dalton Transactions, (39): 7353-7363 2010.

John, A.; Shaikh, M. M.; Ghosh, P.

*Suzuki-Miyaura cross-coupling of aryl chlorides catalyzed by palladium precatalysts of N/O-functionalized pyrazolyl ligands*

Inorganica Chimica Acta, (363): 3113-3121 2010.

Jornet, D.; Bartovsky, P.; Domingo, L. R.; Tormos, R.; Miranda, M. A.

*Experimental and Theoretical Studies on the Mechanism of Photochemical Hydrogen Transfer from 2-Aminobenzimidazole to n pi\* and pi pi\*Aromatic Ketones*

Journal of Physical Chemistry B, (114): 11920-11926 2010.

Joseph, B.; John, S.; Aravindakshan, K. K.; Joseph, A.

*Inhibition of mild steel corrosion in 1 M hydrochloric acid using (E)-4-(2-chlorobenzylideneamino)-6-methyl-3-thioxo-3,4-dihydro-1,2,4-triazin-5(2H)-one (CBMTDT)*  
Indian Journal of Chemical Technology, (17): 425-430 2010.

Justino, G. C.; Vieira, A. J. S. C.

*Antioxidant mechanisms of Quercetin and Myricetin in the gas phase and in solution - a comparison and validation of semi-empirical methods*

Journal of Molecular Modeling, (16): 863-876 2010.

Kalikanda, J.; Li, Z.

*Regioselective glycosylation reactions based on computational predictions*  
Tetrahedron Letters, (51): 1550-1553 2010.

Kalikanda, J.; Li, Z. T.

*Regioselective glycosylation reactions based on computational predictions*  
Tetrahedron Letters, (51): 1550-1553 2010.

Kalinowska, M.; Swislocka, R.; Rzaczynska, Z.; Sienkiewicz, J.; Lewandowski, W.

*Spectroscopic (FT-IR, FT-Raman, UV, H-1, and C-13 NMR) and theoretical studies of m-anisic acid and lithium, sodium, potassium, rubidium, and caesium m-anisates*  
Journal of Physical Organic Chemistry, (23): 37-47 2010.

Kapitan, J.; Dracinsky, M.; Kaminsky, J.; Benda, L.; Bour, P.

*Theoretical Modeling of Magnesium Ion Imprints in the Raman Scattering of Water*  
Journal of Physical Chemistry B, (114): 3574-3582 2010.

Karpinska, G.; Mazurek, A. P.; Dobrowolski, J. C.

*On tautomerism and substituent effect in 8-hydroxyquinoline-derived medicine molecules*  
Journal of Molecular Structure-Theochem, (961): 101-106 2010.

Kasetti, Y.; Patel, N. K.; Sundriyal, S.; Bharatam, P. V.

*Conformational Polymorphism in Sulfonylurea Drugs: Electronic Structure Analysis*  
Journal of Physical Chemistry B, (114): 11603-11611 2010.

Kassaee, M. Z.; Musavi, S. M.; Motamed, E.

*Borepin, Boranorbornadiene and Boranorcaradiene: Substituent Effects on Interconversions at Theoretical Levels*

Journal of Theoretical & Computational Chemistry, (9): 379-392 2010.

Kassaee, M. Z.; Rad, H. A.

*Silicon-carbon vs. carbon nanotubes at DFT: Aromaticity, polarizability, and structural network(s) at various lengths and widths*

Computational Materials Science, (48): 144-149 2010.

Kassaee, M. Z.; Rad, H. A.; Amiri, S. S.

*Carbon-nitrogen nanorings and nanoribbons: a theoretical approach for altering the ground states of cyclacenes and polyacenes*

Monatshefte fur Chemie, (141): 1313-1319 2010.

Katkova, M. A.; Balashova, T. V.; Maleev, A. A.; Illichev, V. A.; Konev, A. N.; Fukin, G. K.; Mitin, A. S.; Ketkov, S. Y.; Bochkarev, M. N.

*Yellow-green organic light-emitting diode based on tris(2-methyl-8-quinolinolate) scandium*  
Synthetic Metals, (160): 2476-2480 2010.

Kaur, D.; Khanna, S.; Kaur, R. P.

*The role of conjugative interactions in acidic and basic character of five membered aromatic heterocyclics*

Journal of Molecular Structure-Theochem, (949): 14-22 2010.

Kaur, D.; Sharma, P.; Bharatam, P. V.

*Importance of selenium in antioxidant behavior of ebselen: A theoretical study*

Journal of Molecular Structure-Theochem, (939): 118-123 2010.

Kaur, P.; Kaur, S.; Kasetti, Y.; Bharatam, P. V.; Singh, K.

*A new colorimetric chemodosimeter for Hg<sup>2+</sup> based on charge-transfer compound of N-methylpyrrole with TCNQ*

Talanta, (83): 644-650 2010.

Kavitha, E.; Sundaraganesan, N.; Sebastian, S.; Kurt, M.

*Molecular structure, anharmonic vibrational frequencies and NBO analysis of naphthalene acetic acid by density functional theory calculations*

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (77): 612-619 2010.

Keiter, R. L.; Ye, P.; Keiter, E. A.; Benson, J. W.; Lin, W.; Brandt, D. E.; Southern, J. S.; Rheingold, A. L.; Guzei, I.; Wheeler, K. A.; Cary, L. W.

*Intramolecular exchange of coordinated and dangling phosphines in pentacarbonyl group 6 complexes of 1,1,2-tris(diphenylphosphino)ethane*

Inorganica Chimica Acta, (364): 176-184 2010.

Keith, J. M.; Tomic, Z. D.; Zaric, S. D.; Hall, M. B.

*Oxygen atom transfer catalysis: Ligand effects on the key reaction barrier in molybdenum (VI) dioxo systems*

Journal of Molecular Catalysis a-Chemical, (324): 15-23 2010.

- Keller, J. W.; Harrod, B. L.; Chowdhury, S. A.  
*Theoretical Study of Formic Acid-Sulfur Dioxide Dimers*  
Journal of Physical Chemistry A, (114): 13182-13188 2010.
- Kemnitz, C. R.; Mackey, J. L.; Loewen, M. J.; Hargrove, J. L.; Lewis, J. L.; Hawkins, W. E.; Nielsen, A. E.  
*Origin of Stability in Branched Alkanes*  
Chemistry-a European Journal, (16): 6942-6949 2010.
- Kempter, V.; Kirchner, B.  
*The role of hydrogen atoms in interactions involving imidazolium-based ionic liquids*  
Journal of Molecular Structure, (972): 22-34 2010.
- Kesharwani, M. K.; Khan, M. A. S.; Bandyopadhyay, T.; Ganguly, B.  
*Solvolysis process of organophosphorus compound P-[2-(dimethylamino)ethyl]-N,N-dimethylphosphonamidic fluoride with simple and alpha-nucleophiles: a DFT study*  
Theoretical Chemistry Accounts, (127): 39-47 2010.
- Khaled, K. F.  
*Studies of iron corrosion inhibition using chemical, electrochemical and computer simulation techniques*  
Electrochimica Acta, (55): 6523-6532 2010.
- Khan, M. A. S.; Kesharwani, M. K.; Bandyopadhyay, T.; Ganguly, B.  
*Remarkable effect of hydroxylamine anion towards the solvolysis of sarin: A DFT study*  
Journal of Molecular Structure-Theochem, (944): 132-136 2010.
- Khedkar, J. K.; Gobre, V. V.; Pinjari, R. V.; Gejji, S. P.  
*Electronic Structure and Normal Vibrations in (+)-Catechin and (-)-Epicatechin Encapsulated beta-Cyclodextrin*  
Journal of Physical Chemistry A, (114): 7725-7732 2010.
- Kheffache, D.; Ouamerali, O.  
*Some physicochemical properties of the antitumor drug thiotepa and its metabolite tepa as obtained by density functional theory (DFT) calculations*  
Journal of Molecular Modeling, (16): 1383-1390 2010.
- Khenkin, A. M.; Efremenko, I.; Weiner, L.; Martin, J. M. L.; Neumann, R.  
*Photochemical Reduction of Carbon Dioxide Catalyzed by a Ruthenium-Substituted Polyoxometalate*  
Chemistry-a European Journal, (16): 1356-1364 2010.
- Khodabandeh, M. H.; Davari, M. D.; Zahedi, M.; Ohanessian, G.  
*Complexation of glycine by manganese (II) in the gas phase: A theoretical study*  
International Journal of Mass Spectrometry, (291): 73-83 2010.
- Khorassani, S. M. H.; Ebrahimi, A.; Maghsoudlou, M. T.; Ghahghayi, Z.; Ghasempour, H.; Kazemian, M. A.

*NMR study and AIM analysis for the ylide rotamers from the reaction between triphenylphosphine and dialkyl acetylenedicarboxylates in the presence of 2-mercaptop-1-methylimidazole*  
Journal of Sulfur Chemistry, (31): 153-160 2010.

Kim, S.-U.; Liu, Y.; Nash, K. M.; Zweier, J. L.; Rockenbauer, A.; Villamena, F. A.  
*Fast Reactivity of a Cyclic Nitrone-Calix[4]pyrrole Conjugate with Superoxide Radical Anion: Theoretical and Experimental Studies*  
Journal of the American Chemical Society, (132): 17157-17173 2010.

Kingsbury, C. A.  
*Transition states in Ei reactions*  
Journal of Physical Organic Chemistry, (23): 513-518 2010.

Kinjo, R.; Donnadieu, B.; Bertrand, G.  
*Isolation of a Carbene-Stabilized Phosphorus Mononitride and Its Radical Cation (PN+center dot)*  
Angewandte Chemie-International Edition, (49): 5930-5933 2010.

Kirchner, B.; Spickermann, C.; Reckien, W.; Schalley, C. A.  
*Uncovering Individual Hydrogen Bonds in Rotaxanes by Frequency Shifts*  
Journal of the American Chemical Society, (132): 484-494 2010.

Kirsch, P.; Bremer, M.  
*Understanding Fluorine Effects in Liquid Crystals*  
Chemphyschem, (11): 357-360 2010.

Kita, Y.; Hayashi, S.; Kinoshita, I.; Tachibana, M.; Tachikawa, M.; Kobayashi, K.; Tanimura, M.  
*First-principles calculation and transmission electron microscopy observation for hydrogen adsorption on carbon nanowalls*  
Journal of Applied Physics, (108) 2010.

Klein, S.; Frenking, G.  
*Carbodiyrides C(ECp\*)(2) (E = B-Tl): Another Class of Theoretically Predicted Divalent Carbon(0) Compounds*  
Angewandte Chemie-International Edition, (49): 7106-7110 2010.

Klein, S.; Tonner, R.; Frenking, G.  
*Carbodicarbones and Related Divalent Carbon(0) Compounds*  
Chemistry-a European Journal, (16): 10160-10170 2010.

Knight, F. R.; Fuller, A. L.; Buehl, M.; Slawin, A. M. Z.; Woollins, J. D.  
*Hypervalent Adducts of Chalcogen-Containing peri-Substituted Naphthalenes; Reactions of Sulfur, Selenium, and Tellurium with Dihalogens*  
Inorganic Chemistry, (49): 7577-7596 2010.

Knight, F. R.; Fuller, A. L.; Buehl, M.; Slawin, A. M. Z.; Woollins, J. D.  
*Sterically Crowded peri-Substituted Naphthalene Phosphines and their P-V Derivatives*  
Chemistry-a European Journal, (16): 7617-7634 2010.

- Knight, F. R.; Fuller, A. L.; Buehl, M.; Slawin, A. M. Z.; Woollins, J. D.  
*Synthetic and Structural Studies of 1,8-Chalcogen Naphthalene Derivatives*  
Chemistry-a European Journal, (16): 7503-7516 2010.
- Knight, F. R.; Fuller, A. L.; Buehl, M.; Slawin, A. M. Z.; Woollins, J. D.  
*Synthetic and Structural Studies of 1-Halo-8-(alkylchalcogeno)naphthalene Derivatives*  
Chemistry-a European Journal, (16): 7605-7616 2010.
- Koide, T.; Furukawa, K.; Shinokubo, H.; Shin, J.-Y.; Kim, K. S.; Kim, D.; Osuka, A.  
*A Stable Non-Kekule Singlet Biradicaloid from meso-Free 5,10,20,25-Tetrakis(Pentafluorophenyl)-Substituted [26]Hexaphyrin(1.1.1.1.1)*  
Journal of the American Chemical Society, (132): 7246-+ 2010.
- Koirala, P.; Willis, M.; Kiran, B.; Kandalam, A. K.; Jena, P.  
*Superhalogen Properties of Fluorinated Coinage Metal Clusters*  
Journal of Physical Chemistry C, (114): 16018-16024 2010.
- Koivisto, J. J.; Kumpulainen, E. T. T.; Koskinen, A. M. P.  
*Conformational ensembles of flexible beta-turn mimetics in DMSO-d(6)*  
Organic & Biomolecular Chemistry, (8): 2103-2116 2010.
- Koizumi, T.-a.; Teratani, T.; Okamoto, K.; Yamamoto, T.; Shimoji, Y.; Kanbara, T.  
*Nickel(II) complexes bearing a pincer ligand containing thioamide units: Comparison between SNS- and SCS-pincer ligands*  
Inorganica Chimica Acta, (363): 2474-2480 2010.
- Koput, J.; Makarewicz, J.  
*Ab initio characterization of the Mg-HF van der Waals complex*  
Journal of Chemical Physics, (133) 2010.
- Korzan, R.; Upton, B.; Turnbull, K.; Seybold, P. G.  
*Quantum Chemical Study of the Energetics and Directionality of Acid-Catalyzed Aromatic Epoxide Ring Openings*  
International Journal of Quantum Chemistry, (110): 2931-2937 2010.
- Koshevoy, I. O.; Karttunen, A. J.; Lin, Y.-C.; Lin, C.-C.; Chou, P.-T.; Tunik, S. P.; Haukka, M.; Pakkanen, T. A.  
*Synthesis, photophysical and theoretical studies of luminescent silver(I)-copper(I) alkynyl-diphosphine complexes*  
Dalton Transactions, (39): 2395-2403 2010.
- Kosmas, A. M.; Papayannis, D. K.  
*Computational characterisation of the charge-transfer and T-shaped molecular complexes of N-methyl imidazoline-2-thione and N-methyl imidazolidine-2-thione with the dihalogens Br-2 and I-2*  
Molecular Simulation, (36): 212-220 2010.
- Kostova, I.; Amalanathan, M.; Joe, I. H.

*Molecular first order hyperpolarizability and vibrational spectral investigation of Warfarin sodium*

Chemical Physics, (378): 88-102 2010.

Kovacs, A.; Nemcsok, D. S.; Kocsis, T.

*Bonding interactions in EDTA complexes*

Journal of Molecular Structure-Theochem, (950): 93-97 2010.

Koyanagi, G. K.; Kapishon, V.; Bohme, D. K.; Zhang, X.; Schwarz, H.

*Reactivity Pattern in the Room-Temperature Activation of NH<sub>3</sub> by the Main-Group Atomic Ions Ga<sup>+</sup>, Ge<sup>+</sup>, As<sup>+</sup> and Se<sup>+</sup>*

European Journal of Inorganic Chemistry: 1516-1521 2010.

Koz, G.; Ozdemir, N.; Astley, D.; Dincer, M.; Astley, S. T.

*Synthesis, spectroscopic and structural characterization of cobalt(II) complex with uracil-containing 2,6-diformylpyridine ligand: Theoretical studies on the ligand and pentagonal-bipyramidal [Co(L)(H<sub>2</sub>O)(2)](2+) and [Zn(L)(H<sub>2</sub>O)(2)](2+) cations*

Journal of Molecular Structure, (966): 39-47 2010.

Kraka, E.; Jooy, H.; Cremer, D.

*A stunning example for a spontaneous reaction with a complex mechanism: the vinylidene-acetylene cycloaddition reaction*

Molecular Physics, (108): 2667-2685 2010.

Krisilov, A. V.; Zon, B. A.

*Electronic Structure and Spectrum of Endofullerene Cation [Ce@C-60](+)*

Optics and Spectroscopy, (109): 833-838 2010.

Kruszynski, R.; Trzesowska-Kruszynska, A.

*Halogen, hydrogen and electrostatic interactions in 2-amino-5-chloro-1,3-benzoxazol-3-ium nitrate and 2-amino-5-chloro-1,3-benzoxazol-3-ium perchlorate*

Acta Crystallographica Section C-Crystal Structure Communications, (66): 449-454 2010.

Krygowski, T. M.; Oziminski, W. P.; Palusiak, M.; Fowler, P. W.; McKenzie, A. D.

*Aromaticity of substituted fulvene derivatives: substituent-dependent ring currents*

Physical Chemistry Chemical Physics, (12): 10740-10745 2010.

Kuchenbecker, D.; Harder, S.; Jansen, G.

*Insight in Structures of Superbulky Metallocenes with the Cp-BIG Ligand: Theoretical Considerations of Decaphenyl Metallocenes*

Zeitschrift fur Anorganische und Allgemeine Chemie, (636): 2257-2261 2010.

Kudinov, A. R.; Zanello, P.; Herber, R. H.; Loginov, D. A.; Vinogradov, M. M.; Vologzhanina, A. V.; Starikova, Z. A.; Corsini, M.; Giorgi, G.; Nowik, I.

*Ferracarborane Benzene Complexes [(eta-9-L-7,8-C<sub>2</sub>B<sub>9</sub>H<sub>10</sub>)Fe(eta-C<sub>6</sub>H<sub>6</sub>)](+) (L = SMe<sub>2</sub>, NMe<sub>3</sub>):*

*Synthesis, Reactivity, Electrochemistry, Mossbauer Effect Studies, and Bonding*

Organometallics, (29): 2260-2271 2010.

- Kumar, N. V. S.; Sharma, P.; Singh, H.; Koley, D.; Roy, S.; Chakraborty, T. K.  
*Preferential mode of cyclization of tetrahydrofuran amino acids containing peptides: some theoretical insights*  
Journal of Physical Organic Chemistry, (23): 238-245 2010.
- Kuprat, M.; Kuzora, R.; Lehmann, M.; Schulz, A.; Villinger, A.; Wustrack, R.  
*Silver tetrakis(hexafluoroisopropoxy)aluminate as hexafluoroisopropyl transfer reagent for the chlorine/hexafluoroisopropyl exchange in imino phosphanes*  
Journal of Organometallic Chemistry, (695): 1006-1011 2010.
- Kurczab, R.; Mitoraj, M. P.; Michalak, A.; Ziegler, T.  
*Theoretical Analysis of the Resonance Assisted Hydrogen Bond Based on the Combined Extended Transition State Method and Natural Orbitals for Chemical Valence Scheme*  
Journal of Physical Chemistry A, (114): 8581-8590 2010.
- Kurian, R.; Filatov, M.  
*Calibration of Fe-57 isomer shift from ab initio calculations: can theory and experiment reach an agreement?*  
Physical Chemistry Chemical Physics, (12): 2758-2762 2010.
- Kurouchi, H.; Sugimoto, H.; Otani, Y.; Ohwada, T.  
*Cyclization of Arylacetoacetates to Indene and Dihydronaphthalene Derivatives in Strong Acids. Evidence for Involvement of Further Protonation of O,O-Diprotonated beta-Ketoester, Leading to Enhancement of Cyclization*  
Journal of the American Chemical Society, (132): 807-815 2010.
- Kus, N.; Reva, I.; Fausto, R.  
*Photoisomerization and Photochemistry of Matrix-Isolated 3-Furaldehyde*  
Journal of Physical Chemistry A, (114): 12427-12436 2010.
- Kusama, H.; Sugihara, H.; Sayama, K.  
*Simultaneous Interactions of Ru Dye with Iodide Ions and Nitrogen-Containing Heterocycles in Dye-Sensitized Solar Cells*  
Journal of Physical Chemistry C, (114): 11335-11341 2010.
- Kusama, H.; Sugihara, H.; Sayama, K.  
*Simultaneous Interactions of Ru Dye with Iodide Ions and Nitrogen-Containing Heterocycles in Dye-Sensitized Solar Cells*  
Journal of Physical Chemistry C, (114): 11335-11341 2010.
- Kuta, J.; Clark, A. E.  
*Trends in Aqueous Hydration Across the 4f Period Assessed by Reliable Computational Methods*  
Inorganic Chemistry, (49): 7808-7817 2010.
- Kuwabara, J.; Munezawa, G.; Okamoto, K.; Kanbara, T.  
*Palladium(II) and platinum(II) complexes bearing a kappa(SCS)-S-3 pincer ligand with an azulene unit*  
Dalton Transactions, (39): 6255-6261 2010.

- Kuwabara, J.; Yamagata, T.; Kanbara, T.  
*Solid-state structure and optical properties of highly fluorescent diketopyrrolopyrrole derivatives synthesized by cross-coupling reaction*  
Tetrahedron, (66): 3736-3741 2010.
- Kuznetsov, M. L.; Bokach, N. A.; Kharlampidi, D. D.; Medvedev, Y. N.; Kukushkin, V. Y.; Dementiev, A. I.  
*Theoretical study of nucleophilic addition of amines to organic nitriles*  
Russian Journal of General Chemistry, (80): 458-467 2010.
- Kuznetsov, M. L.; Kukushkin, V. Y.; Pombeiro, A. J. L.  
*Comparative Theoretical Study of 1,3-Dipolar Cycloadditions of Allyl-Anion Type Dipoles to Free and Pt-Bound Nitriles*  
Journal of Organic Chemistry, (75): 1474-1490 2010.
- Kwit, M.; Gawronski, J.; Boyd, D. R.; Sharma, N. D.; Kaik, M.  
*Circular dichroism, optical rotation and absolute configuration of 2-cyclohexenone-cis-diol type phenol metabolites: redefining the role of substituents and 2-cyclohexenone conformation in electronic circular dichroism spectra*  
Organic & Biomolecular Chemistry, (8): 5635-5645 2010.
- Lage, M. L.; Fernandez, I.; Mancheno, M. J.; Gomez-Gallego, M.; Sierra, M. A.  
*The Electronic Structure and Photochemistry of Group 6 Bimetallic (Fischer) Carbene Complexes: Beyond the Photocarbonylation Reaction*  
Chemistry-a European Journal, (16): 6616-6624 2010.
- Lai, C. H.; Chou, P. T.  
*A systematic study of the stabilities of cyclic boryl anions*  
Journal of Molecular Modeling, (16): 713-723 2010.
- Lai, C.-H.; Chou, P.-T.  
*A systematic study of the stabilities of cyclic boryl anions*  
Journal of Molecular Modeling, (16): 713-723 2010.
- Lamsabhi, A. M.; Mo, O.; Yanez, M.  
*Serine-Ca<sup>2+</sup> versus serine-Cu<sup>2+</sup> complexes - A theoretical perspective*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 759-768 2010.
- Langer, V.; Mach, P.; Smrcok, L.; Milata, V.; Plevova, K.  
*2-{{(3-Fluorophenyl)amino)methylidene}-3-oxobutanenitrile and 5-{{(3-fluorophenyl)amino)methylidene}-2,2-dimethyl-1,3-dioxane-4,6-dion e: X-ray and DFT studies*  
Acta Crystallographica Section C-Crystal Structure Communications, (66): o392-o395 2010.
- Lankau, T.; Yu, C.-H.  
*A Model Study of the Efficiency of the Asp-His-Ser Triad*  
Journal of Computational Chemistry, (31): 1853-1859 2010.

Larionova, M.; Spengler, I.; Nogueiras, C.; Quijano, L.; Ramirez-Gualito, K.; Cortes-Guzman, F.; Cuevas, G.; Calderon, J. S.

*A C-Glycosylflavone from Piper ossanum, a Compound Conformationally Controlled by CH/pi and Other Weak Intramolecular Interactions*

Journal of Natural Products, (73): 1623-1627 2010.

Larkin, J. D.; Fossey, J. S.; James, T. D.; Brooks, B. R.; Bock, C. W.

*A Computational Investigation of the Nitrogen-Boron Interaction in o-(N,N-Dialkylaminomethyl)arylboronate Systems*

Journal of Physical Chemistry A, (114): 12531-12539 2010.

Laskavy, A.; Shimon, L. J. W.; Konstantinovski, L.; Iron, M. A.; Neumann, R.

*Activation of Molecular Oxygen by a Dioxygenase Pathway by a Ruthenium Bis-bipyridine Compound with a Proximal Selenium Site*

Journal of the American Chemical Society, (132): 517-523 2010.

Lattanzi, V.; Thorwirth, S.; Halfen, D. T.; Mueck, L. A.; Ziurys, L. M.; Thaddeus, P.; Gauss, J.; McCarthy, M. C.

*Bonding in the Heavy Analogue of Hydrogen Cyanide: The Curious Case of Bridged HPSi*

Angewandte Chemie-International Edition, (49): 5661-5664 2010.

Laurence, C.; Graton, J.; Berthelot, M.; Besseau, F.; Le Questel, J.-Y.; Lucon, M.; Ouvrard, C.; Planchat, A.; Renault, E.

*An Enthalpic Scale of Hydrogen-Bond Basicity. 4. Carbon pi Bases, Oxygen Bases, and Miscellaneous Second-Row, Third-Row, and Fourth-Row Bases and a Survey of the 4-Fluorophenol Affinity Scale*

Journal of Organic Chemistry, (75): 4105-4123 2010.

Lavenda, B. H.

*New Perspective on Thermodynamics*

New Perspective on Thermodynamics: 1-207 2010.

Lavoie, N.; Gorelsky, S. I.; Liu, Z.; Burchell, T. J.; Yap, G. P. A.; Richeson, D. S.

*Disubstituted 1,8-Diamidonaphthalene Ligands as a Flexible, Responsive, and Reactive Framework for Tantalum Complexes*

Inorganic Chemistry, (49): 5231-5240 2010.

Lazareva, N. F.; Shainyan, B. A.; Kleinpeter, E.

*4-Alkyl-2,2,6,6-tetramethyl-1,4,2,6-oxaazadisilinanes: synthesis, structure, and conformational analysis*

Journal of Physical Organic Chemistry, (23): 84-89 2010.

Leach, S.; Champion, N.; Jochims, H.-W.; Baumgaertel, H.

*Photoionization mass spectrometric studies of N-methyl formamide and N, N'-dimethyl formamide in the 7-18 eV photon energy range*

Chemical Physics, (376): 10-22 2010.

Ledesma, A. E.; Contreras, C.; Svoboda, J.; Vektariane, A.; Brandan, S. A.

*Theoretical structures and experimental vibrational spectra of isomeric benzofused thieno [3,2-b] furan compounds*  
Journal of Molecular Structure, (967): 159-165 2010.

Ledesma, A. E.; Zinczuk, J.; Lopez Gonzalez, J. J.; Ben Altabef, A.; Brandan, S. A.  
*Structural, vibrational spectra and normal coordinate analysis for two tautomers of 4(5)-(2'-furyl)-imidazole*  
Journal of Raman Spectroscopy, (41): 587-597 2010.

Lehmann, S. B. C.; Roatsch, M.; Schoeppke, M.; Kirchner, B.  
*On the physical origin of the cation-anion intermediate bond in ionic liquids Part I. Placing a (weak) hydrogen bond between two charges*  
Physical Chemistry Chemical Physics, (12): 7473-7486 2010.

Lesarri, A.; Vega-Toribio, A.; Suenram, R. D.; Brugh, D. J.; Grabow, J.-U.  
*The conformational landscape of the volatile anesthetic sevoflurane*  
Physical Chemistry Chemical Physics, (12): 9624-9631 2010.

Lesarri, A.; Vega-Toribio, A.; Suenram, R. D.; Brugh, D. J.; Grabow, J. U.  
*The conformational landscape of the volatile anesthetic sevoflurane*  
Physical Chemistry Chemical Physics, (12): 9624-9631 2010.

Less, R. J.; McPartlin, M.; Rawson, J. M.; Wood, P. T.; Wright, D. S.  
*A Simple Approach to Coordination Compounds of the Pentacyanocyclopentadienide Anion*  
Chemistry-a European Journal, (16): 13723-13728 2010.

Lever, A. B. P.  
*Electronic characteristics of an extensive series of ruthenium complexes with the non-innocent o-benzoquinonediimine ligand: A pedagogical approach*  
Coordination Chemistry Reviews, (254): 1397-1405 2010.

Li, F.-X.; Gorham, K.; Armentrout, P. B.  
*Oxidation of Atomic Gold Ions: Thermochemistry for the Activation of O-2 and N2O by Au+ (S-1/0) and D-3)*  
Journal of Physical Chemistry A, (114): 11043-11052 2010.

Li, H.; Li, C.; Fan, H.; Yang, J.  
*Studies on electronic structures, energetics, and electron affinities of transition metal-benzene complexes and their anions with density functional theory*  
Journal of Molecular Structure-Theochem, (952): 67-73 2010.

Li, H.; Zhang, L.; Hu, Y.  
*Density Functional Theory Study on the Relationship between Polymerization Activity and Substituent Electronic Effect of Polyolefin Catalysts*  
Chinese Journal of Catalysis, (31): 1127-1131 2010.

Li, H.; Zhao, L.; Lu, G.; Mo, Y.; Wang, Z.-X.

*Insight into the relative reactivity of "Frustrated Lewis pairs" and stable carbenes in activating H<sub>2</sub> and CH<sub>4</sub>: A comparative computational study*  
Physical Chemistry Chemical Physics, (12): 5268-5275 2010.

Li, J.  
*A multivariate relationship for the impact sensitivities of energetic N-nitrocompounds based on bond dissociation energy*  
Journal of Hazardous materials, (174): 728-733 2010.

Li, J.; Merkel, S.; Henn, J.; Meindl, K.; Doering, A.; Roesky, H. W.; Ghadwal, R. S.; Stalke, D.  
*Lewis-Base-Stabilized Dichlorosilylene: A Two-Electron sigma-Donor Ligand*  
Inorganic Chemistry, (49): 775-777 2010.

Li, N.; Xie, Y.; King, R. B.; Schaefer, H. F., III  
*Diverse Roles of Hydrogen in Rhenium Carbonyl Chemistry: Hydrides, Dihydrogen Complexes, and a Formyl Derivative*  
Journal of Physical Chemistry A, (114): 11670-11680 2010.

Li, P.; Ma, Z. Y.; Wang, W. H.; Shen, Z. T.; Bi, S. W.; Sun, H. T.; Bu, Y. X.  
*Coupling Interactions between Sulfurous Acid and the Hydroperoxyl Radical*  
Chemphyschem, (11): 696-705 2010.

Li, P.; Ma, Z.-Y.; Wang, W.-H.; Shen, Z.-T.; Bi, S.-W.; Sun, H.-T.; Bu, Y.-X.  
*Coupling Interactions between Sulfurous Acid and the Hydroperoxyl Radical*  
Chemphyschem, (11): 696-705 2010.

Li, P.; Shen, Z.; Wang, W.; Ma, Z.; Bi, S.; Sun, H.; Bu, Y.  
*The capture of H-center dot and (OH)-O-center dot radicals by vitamin C and implications for the new source for the formation of the anion free radical*  
Physical Chemistry Chemical Physics, (12): 5256-5267 2010.

Li, Q.; Jing, B.; Liu, Z.; Li, W.; Cheng, J.; Gong, B.; Sun, J.  
*Competition and cooperativity between hydrogen bond and sigma-hole bond in SCS-(HF)(n) (n=1 and 2) systems*  
Journal of Molecular Structure-Theochem, (952): 90-95 2010.

Li, Q.; Jing, B.; Liu, Z.; Li, W.; Cheng, J.; Gong, B.; Sun, J.  
*Surprising enhancing effect of methyl group on the strength of O center dot center dot center dot XF and S center dot center dot center dot XF (X=Cl and Br) halogen bonds*  
Journal of Chemical Physics, (133) 2010.

Li, Q.; Liu, Z.; Jing, B.; Li, W.; Cheng, J.; Gong, B.; Sun, J.  
*Large blue shift of the H-Ar stretching frequency in hydrogen- and halogen-bonded complexes of HArF with dihalogen molecules*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (77): 506-511 2010.

Li, Q.; Xu, X.; Liu, T.; Jing, B.; Li, W.; Cheng, J.; Gong, B.; Sun, J.

*Competition between hydrogen bond and halogen bond in complexes of formaldehyde with hypohalous acids*

Physical Chemistry Chemical Physics, (12): 6837-6843 2010.

Li, Q.; Yuan, H.; Jing, B.; Liu, Z.; Li, W.; Cheng, J.; Gong, B.; Sun, J.

*Theoretical study of halogen-hydride halogen bonds in F3CL center dot center dot center dot HM (L = Cl, Br; M = Li, BeH, MgH) complexes*  
Molecular Physics, (108): 611-617 2010.

Li, Q.-G.; Xue, Y.; Guo, Y.; Yan, G.-S.

*Phosphonylation and Activity Loss Mechanism of the Catalytic Triad of Fatty Acid Amide Hydrolase: Theoretical Study of a Model System*  
Acta Physico-Chimica Sinica, (26): 1965-1975 2010.

Li, Q.-Z.; Dong, X.; Jing, B.; Li, W.-Z.; Cheng, J.-B.; Gong, B.-A.; Yu, Z.-W.

*A New Unconventional Halogen Bond C-X center dot center dot center dot H-M Between HCCX (X = Cl and Br) and HMH (M = Be and Mg): An Ab Initio Study*  
Journal of Computational Chemistry, (31): 1662-1669 2010.

Li, W.-W.; Hou, R.-B.; Sun, Y.-L.

*Characteristics of One Electron Redox Behavior of Hydrophobic Amino Acids in Gas Phase*  
Acta Physico-Chimica Sinica, (26): 2772-2778 2010.

Li, X.; Cao, X.

*Theoretical treatment of MAr42+ (M = Cu, Ag and Au)*  
Molecular Physics, (108): 2115-2119 2010.

Li, X.; Wu, S.; Zhou, C.; Zhao, Y.

*Theoretical Investigation on Structures and Stabilities of CuXenZ (n=1-3, Z = -1, 0,+1) Clusters*  
Australian Journal of Chemistry, (63): 474-478 2010.

Li, X.; Zhang, R.; Zhang, X.

*Computational study of imidazole derivative as high energetic materials*  
Journal of Hazardous materials, (183): 622-631 2010.

Li, X.-H.; Tang, Z.-X.; Zhang, X.-Z.

*Natural Bond Orbital Analysis of Some S-Nitrosothiols Biological Molecules*  
International Journal of Quantum Chemistry, (110): 1565-1572 2010.

Li, X.-H.; Yin, G.-X.; Zhang, X.-Z.

*Natural bond orbital (NBO) population analysis of some benzyl nitrites*  
Journal of Molecular Structure-Theochem, (957): 61-65 2010.

Li, Y.; Zou, J.-J.; Zhang, X.; Wang, L.; Mi, Z.

*Product distribution of tricyclopentadiene from cycloaddition of dicyclopentadiene and cyclopentadiene: A theoretical and experimental study*  
Fuel, (89): 2522-2527 2010.

Li, Y. M.; Zhou, X. M.; Tang, K.; Qin, M.; Zhou, Z. Y.

*DFT studies on hydrogen bonded complexes of thymine with formamide*

Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (49): 145-150 2010.

Li, Y.-m.; Zhou, X.-m.; Tang, K.; Qin, M.; Zhou, Z.-y.

*DFT studies on hydrogen bonded complexes of thymine with formamide*

Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (49): 145-150 2010.

Li, Z.; Shi, X.; Tang, H.; Zhang, J.

*Theoretical study of the interaction mechanism of single-electron halogen bond complexes H3C center dot center dot center dot Br-Y (Y = H, CN, NC, CCH, C2H3)*

Science China-Chemistry, (53): 216-225 2010.

Li, Z.-F.; Zhang, Y.-Q.; Li, H.-X.; Zhu, Y.-C.; Yang, S.

*Theoretical observations of the single-electron lithium system H-Be center dot center dot center dot Li-Y (Y = H, OH, F, CCH, CN and NC)*

Journal of Molecular Structure-Theochem, (958): 48-51 2010.

Li, Z.-M.; Xiong, Z.; Dai, L.-L.

*Calculation of geometrically active atomic state*

Acta Physica Sinica, (59): 7824-7829 2010.

Liang, J.-X.; Geng, Z.-Y.; Wang, Y.-C.

*Reactivity of hydrogen abstraction in CH2Cl2 by CHX center dot- (X = F, Cl, Br, I) from a theoretical viewpoint*

Journal of Molecular Structure-Theochem, (958): 15-20 2010.

Liang, X.; Pu, X.; Tian, A.

*Theoretical Studies on Structures and Properties of Pentrazine Derivations Substituted by Substituent Groups Containing Nitrogen*

Acta Chimica Sinica, (68): 1568-1576 2010.

Lim, Y. M.; Park, C. H.; Yoon, S. J.; Cho, H. M.; Lee, M. E.; Baeck, K. K.

*New Synthetic Routes for Silaheterocycles: Reactions of a Chlorosilylenoid with Aldehydes*  
Organometallics, (29): 1355-1361 2010.

Lin, P.-H.; Gorelsky, S.; Savard, D.; Burchell, T. J.; Wernsdorfer, W.; Clerac, R.; Murugesu, M.

*Synthesis, characterisation and computational studies on a novel one-dimensional arrangement of Schiff-base Mn-3 single-molecule magnet*  
Dalton Transactions, (39): 7650-7658 2010.

Ling, Y.; Mills, C.; Weber, R.; Yang, L.; Zhang, Y.

*NMR, IR/Raman, and Structural Properties in HNO and RNO (R = Alkyl and Aryl)*

*Metalloporphyrins with Implication for the HNO-Myoglobin Complex*

Journal of the American Chemical Society, (132): 1583-1591 2010.

- Liu, A.; Wu, D.; Jia, D.; Liu, L.  
*Theoretical Studies on Geometry, Solvent Effect, and Photochromic Mechanism of Two Bis-Heterocyclic Compounds Containing Pyrazolone Ring*  
International Journal of Quantum Chemistry, (110): 1360-1367 2010.
- Liu, B.-Y.; Liu, Z.; Han, G.-C.; Li, Y.-H.  
*Synthesis, spectroscopic properties, crystal structure and density functional studies of Cu(II) complex with 2-((dehydroabietylamine)methyl)-6-methoxyphenol*  
Journal of Molecular Structure, (975): 194-199 2010.
- Liu, D.; Zhong, C.  
*Characterization of Lewis Acid Sites in Metal-Organic Frameworks Using Density Functional Theory*  
Journal of Physical Chemistry Letters, (1): 97-101 2010.
- Liu, F.-L.; Liu, X.  
*C<sub>58</sub>Xe: A heterofullerene molecule containing a xenon atom*  
Chemical Physics Letters, (493): 328-332 2010.
- Liu, H.; Chen, Y.-Q.; Yang, Y.-Q.  
*Inverse Hydrogen Bond between Silicane and AB-Type Interhalogen Compounds*  
Acta Physico-Chimica Sinica, (26): 2286-2291 2010.
- Liu, J.; Chen, D.; Zhang, G.; Zhang, Y.; Zhang, H.; Mi, S.; Shen, G.  
*On the origin of decomposition of triphenyl phosphite ozonide accelerated by ammonia or pyridine water solution*  
Journal of Molecular Structure-Theochem, (948): 71-77 2010.
- Liu, J.-X.; Zhang, X.-G.; Duan, Z.-Y.; Liu, X.-L.  
*NO<sub>x</sub> Molecule Adsorption in [Ag]-MAPO-5 (M=Si, Ti) Molecular Sieves*  
Acta Physico-Chimica Sinica, (26): 2679-2685 2010.
- Liu, L. V.; Tian, W. Q.; Chen, Y. K.; Zhang, Y. A.; Wang, Y. A.  
*Theoretical studies on structures, C-13 NMR chemical shifts, aromaticity, and chemical reactivity of finite-length open-ended armchair single-walled carbon nanotubes*  
Nanoscale, (2): 254-261 2010.
- Liu, P.; Liu, J.; Zhang, D.; Zhang, C.  
*A Comparative Theoretical Study of the Reactivities of the Al<sup>+</sup> and Cu<sup>+</sup> Ions Toward Methylamine and Dimethylamine*  
International Journal of Quantum Chemistry, (110): 1583-1593 2010.
- Liu, S.; Hu, H.; Pederset, L. G.  
*Steric, Quantum, and Electrostatic Effects on S(N)2 Reaction Barriers in Gas Phase*  
Journal of Physical Chemistry A, (114): 5913-5918 2010.
- Liu, S.-N.; Cao, D.-L.; Ren, F.-D.; Ren, J.

*Theoretical Investigations on the Structures and Properties of the Side-on Complexes B-2(N-2)(2) and Monocyclic B-n(N-2)(n)(m) (n=3 similar to 6, m =-1 similar to+2)*  
Chinese Journal of Structural Chemistry, (29): 1459-1466 2010.

Liu, T.; Liu, G.-D.; Yu, Z.-Y.  
*Ab initio study of hydrogen bond complexes of ring compounds containing the H2N-C=Y moiety with water*  
Central European Journal of Chemistry, (8): 1115-1124 2010.

Liu, T.; Yu, Z.-Y.  
*Experimental and theoretical study on the supramolecular complexes of 15-crown-5 with adrenaline*  
Bioorganic & Medicinal Chemistry Letters, (20): 4845-4849 2010.

Liu, Y.; Shi, X.; Tang, H.; Liu, X.; Yuan, K.; Zhang, J.; Zhang, J.  
*Co-Existing Lithium Bonding and Hydrogen Bonding Interactions between CH3SH and CH3SLi*  
Acta Chimica Sinica, (68): 493-500 2010.

Long, S.; Li, T.  
*Enforcing Molecule's pi-Conjugation and Consequent Formation of the Acid-Acid Homosynthon over the Acid-Pyridine Heterosynthon in 2-Anilinonicotinic Acids*  
Crystal Growth & Design, (10): 2465-2469 2010.

Lopez, R.; Isabel Menendez, M.; Santander-Nelli, M.; Cardenas-Jiron, G. I.  
*A theoretical investigation on the spectroscopic properties and photosensitizing capability of 5, 10, 15, 20-tetraphenylsapphyrin and 5, 10, 15, 20-tetraphenyl-26,28-diheterosapphyrins with two O, S, or Se Atoms*  
Theoretical Chemistry Accounts, (127): 475-484 2010.

Lorena Picone, A.; Della Vedova, C. O.; Willner, H.; Downs, A. J.; Romano, R. M.  
*Experimental and theoretical characterization of molecular complexes formed between OCS and XY molecules (X, Y = F, Cl and Br) and their role in photochemical matrix reactions*  
Physical Chemistry Chemical Physics, (12): 563-571 2010.

Lorena Picone, A.; Romano, R. M.  
*Infrared matrix-isolation studies of the CS2 center dot center dot center dot HCl molecular complex*  
Journal of Molecular Structure, (978): 187-190 2010.

Lou, X.; Gao, H.; Wang, W.; Xu, C.; Zhang, H.; Zhang, Z.  
*A theoretical study of the atomic hydrogen binding on small AgnCum (n plus m <= 5) clusters*  
Journal of Molecular Structure-Theochem, (959): 75-79 2010.

Lu, B.-M.; Jin, X.-Y.; Tang, J.; Bi, S.-P.  
*DFT studies of Al-O Raman vibrational frequencies for aquated aluminium species*  
Journal of Molecular Structure, (982): 9-15 2010.

Lu, H.-Z.; Feng, Z.-G.; Li, C.; Yuan, H.-Z.; Qin, Z.-H.

*Electronic Structure Comparison between Pyrimorph and Its Phenyl Analog*  
Acta Physico-Chimica Sinica, (26): 1623-1628 2010.

Lukowski, M. A.; Choi, D. J.; Milletti, M. C.

*Substrate Binding and Kinetic Aspects of the Peroxidation Reaction of Four Polyunsaturated Fatty Acids in the COX Active Site of PGHS-1*  
Letters in Drug Design & Discovery, (7): 88-97 2010.

Lumb, J.-P.; Krinsky, J. L.; Trauner, D.

*Theoretical Investigation of the Rubicordifolin Cascade*  
Organic Letters, (12): 5162-5165 2010.

Luo, D.; Zhang, N.; Hong, S.; Wu, H.; Liu, Z.

*Complexes in the Photocatalytic Reaction of CO<sub>2</sub> and H<sub>2</sub>O: Theoretical Studies*  
International Journal of Molecular Sciences, (11): 2792-2804 2010.

Luo, S.-S.; Qiu, Y.-Q.; Liu, C.-G.; Sun, S.-L.; Wang, R.-S.

*Computational Study on Nonlinear Optical Properties of Lambda-Shaped Molecules with Six-membered Carboatomic Ring of Symmetrical Substituent*  
Chemical Journal of Chinese Universities-Chinese, (31): 1436-1441 2010.

Lv, G.; Chen, Z.; Zheng, J.; Wei, F.; Jiang, H.; Zhang, R.; Wang, X.

*Theoretical study of the interaction pattern and the binding affinity between procaine and DNA bases*  
Journal of Molecular Structure-Theochem, (939): 44-52 2010.

Lv, G.; Wei, F.; Li, Q.; Shen, Q.; Jiang, H.; Zhou, Y.; Wang, X.

*DFT Study on the Interactions Between Au-n (n=2 ... 4) and Adenine*  
Journal of Nanoscience and Nanotechnology, (10): 809-818 2010.

Lv, L.; Wang, Y.; Wang, Q.; Liu, H.

*Why is Pt-4(+) the Least Efficient Cationic Cluster in Activating the C-H Bond in Methane? Two-State Reaction Computational Investigation*  
Journal of Physical Chemistry C, (114): 17610-17620 2010.

Lv, L. L.; Wang, Y. C.; Liu, H. W.; Wang, Q.

*Theoretical study of spin-orbit coupling and kinetics in spin-forbidden reaction between Ta(NH<sub>2</sub>)<sub>3</sub> and N<sub>2</sub>O*  
Theoretical Chemistry Accounts, (127): 507-517 2010.

Lyalin, A.; Taketsugu, T.

*Reactant-Promoted Oxygen Dissociation on Gold Clusters*  
Journal of Physical Chemistry Letters, (1): 1752-1757 2010.

Ma, F.; Li, Z.-R.; Zhou, Z.-J.; Wu, D.; Li, Y.; Wang, Y.-F.; Li, Z.-S.

*Modulated Nonlinear Optical Responses and Charge Transfer Transition in Endohedral Fullerene Dimers Na@C<sub>60</sub>C<sub>60</sub>@F with n-Fold Covalent Bond (n=1, 2, 5, and 6) and Long Range Ion Bond*  
Journal of Physical Chemistry C, (114): 11242-11247 2010.

- Ma, F.; Zhou, Z. J.; Li, Z. R.; Wu, D.; Li, Y.; Li, Z. S.  
*Lithium salt of end-substituted nanotube: Structure and large nonlinear optical property*  
Chemical Physics Letters, (488): 182-186 2010.
- Ma, F.; Zhou, Z.-J.; Li, Z.-R.; Wu, D.; Li, Y.; Li, Z.-S.  
*Lithium salt of end-substituted nanotube: Structure and large nonlinear optical property*  
Chemical Physics Letters, (488): 182-186 2010.
- Ma, R.; Cui, H.; Guo, P.; Yang, L.; Guo, L.; Zhang, X.; Liu, G.  
*Influence of the central metal on the structural, electronic, and spectroscopic properties of naphthalocyanine complexes: density functional theory calculations*  
Transition Metal Chemistry, (35): 1005-1012 2010.
- Madzhidov, T. I.; Chmutova, G. A.  
*The nature of hydrogen bonds with divalent selenium compounds*  
Journal of Molecular Structure-Theochem, (959): 1-7 2010.
- Mahdavian, M.; Ashhari, S.  
*Corrosion inhibition performance of 2-mercaptobenzimidazole and 2-mercaptobenzoxazole compounds for protection of mild steel in hydrochloric acid solution*  
Electrochimica Acta, (55): 1720-1724 2010.
- Makal, A. M.; Plazuk, D.; Zakrzewski, J.; Misterkiewicz, B.; Wozniak, K.  
*Experimental Charge Density Analysis of Symmetrically Substituted Ferrocene Derivatives*  
Inorganic Chemistry, (49): 4046-4059 2010.
- Maldonado, A.; Mora, J. R.; Cordova, T.; Chuchani, G.  
*Density functional theory calculations of the gas-phase elimination kinetics of 2-(dimethylamino)ethyl chloride and ethyl chloride*  
Journal of Molecular Structure-Theochem, (961): 55-61 2010.
- Malecki, J. G.; Switlicka, A.; Gron, T.; Balandia, M.  
*Correlation between crystal symmetry and the splitting of d orbital in the thiocyanate nickel(II) complexes*  
Polyhedron, (29): 3198-3206 2010.
- Mandal, A.; Prakash, M.; Kumar, R. M.; Parthasarathi, R.; Subramanian, V.  
*Ab Initio and DFT Studies on Methanol-Water Clusters*  
Journal of Physical Chemistry A, (114): 2250-2258 2010.
- Manz, T. A.; Sholl, D. S.  
*Chemically Meaningful Atomic Charges That Reproduce the Electrostatic Potential in Periodic and Nonperiodic Materials*  
Journal of Chemical Theory and Computation, (6): 2455-2468 2010.
- Marek, R.; Kristkova, A.; Malinakova, K.; Tousek, J.; Marek, J.; Hocek, M.; Malkina, O. L.; Malkin, V. G.

*Interpretation of Indirect Nuclear Spin-Spin Couplings in Isomers of Adenine: Novel Approach to Analyze Coupling Electron Deformation Density Using Localized Molecular Orbitals*  
Journal of Physical Chemistry A, (114): 6689-6700 2010.

Marincean, S.; Jackson, J. E.  
*Can Hydridic-to-Protonic Hydrogen Bonds Catalyze Hydride Transfers in Biological Systems?*  
Journal of Physical Chemistry A, (114): 13376-13380 2010.

Markova, N.; Enchev, V.; Ivanova, G.  
*Tautomeric Equilibria of 5-Fluorouracil Anionic Species in Water*  
Journal of Physical Chemistry A, (114): 13154-13162 2010.

Markovic, S.; Joksovic, M. D.; Bombicz, P.; Leovac, V. M.; Markovic, V.; Joksovic, L.  
*Theoretical study on structural and mechanistic aspects of synthesis of a 3-aminopyrazole derivative*  
Tetrahedron, (66): 6205-6211 2010.

Markovic, Z. S.; Manojlovic, N. T.  
*Analytical characterization of lichenanthrone in lichen: HPLC, UV spectroscopic, and DFT analysis of lichenanthrone extracted from Laurera benguelensis (Mull. Arg.) Zahlbr*  
Monatshefte fur Chemie, (141): 945-952 2010.

Marquez, E.; Dominguez, R. M.; Mora, J. R.; Cordova, T.; Chuchani, G.  
*Experimental and Theoretical Studies of the Homogeneous, Unimolecular Gas-Phase Elimination Kinetics of Trimethyl Orthovalerate and Trimethyl Orthochloroacetate*  
Journal of Physical Chemistry A, (114): 4203-4209 2010.

Martinez-Guajardo, G.; Donald, K. J.; Wittmaack, B. K.; Angel Vazquez, M.; Merino, G.  
*Shorter Still: Compressing C-C Single Bonds*  
Organic Letters, (12): 4058-4061 2010.

Mata, R. A.; Costa Cabral, B. J.  
*QM/MM Approaches to the Electronic Spectra of Hydrogen-Bonding Systems with Connection to Many-Body Decomposition Schemes*  
Advances in Quantum Chemistry, Vol 59, (59): 99-144 2010.

Matos, M. A. R.; Sousa, C. C. S.; Morais, V. M. F.  
*Thermochemistry of chromone- and coumarin-3-carboxylic acid*  
Journal of Thermal Analysis and Calorimetry, (100): 519-526 2010.

Matsugi, M.; Nakamura, S.; Kunda, Y.; Sugiyama, Y.; Shioiri, T.  
*Pronounced rate enhancements in condensation reactions attributed to the fluorous tag in modified Mukaiyama reagents*  
Tetrahedron Letters, (51): 133-135 2010.

Mayer, I.  
*On the promotion energy of an atom in a molecule*  
Chemical Physics Letters, (498): 366-369 2010.

- Mazzone, G.; Russo, N.; Sicilia, E.  
*Gold(I)-Catalyzed Hydration of 1,2-Diphenylacetylene: Computational Insights*  
Journal of Chemical Theory and Computation, (6): 2782-2789 2010.
- McDowell, S. A. C.; Price, K. P.  
*A comparative computational study of novel X-Be-N-2-Li and X-Mg-N-2-Li species (X = F, Cl, Br)*  
Journal of Molecular Structure-Theochem, (962): 85-89 2010.
- McDowell, S. A. C.; Thakkar, A. J.  
*A Simple Model of Hydrogen Bonding With Particular Application to Trends in Hydrogen-Bonded Dimers*  
International Journal of Quantum Chemistry, (110): 1506-1513 2010.
- Mebs, S.; Grabowsky, S.; Foerster, D.; Kickbusch, R.; Hartl, M.; Daemen, L. L.; Morgenroth, W.; Luger, P.; Paulus, B.; Lentz, D.  
*Charge Transfer via the Dative N-B Bond and Dihydrogen Contacts. Experimental and Theoretical Electron Density Studies of Small Lewis Acid-Base Adducts*  
Journal of Physical Chemistry A, (114): 10185-10196 2010.
- Medved, M.; Budzak, S.; Cernusak, I.  
*High second-order NLO responses of dehydrogenated hydrogen cyanide borane(1) oligomers*  
Journal of Molecular Structure-Theochem, (961): 66-72 2010.
- Mehdi, A.; Adane, L.; Patel, D. S.; Bharatam, P. V.  
*Electronic Structure and Reactivity of Guanylthiourea: A Quantum Chemical Study*  
Journal of Computational Chemistry, (31): 1259-1267 2010.
- Memarian, H. R.; Sabzyan, H.; Farhadi, A.  
*DFT study of the molecular structure of 3,4-dihydropyrimidin-2(1H)-ones*  
Monatshefte fur Chemie, (141): 1203-1212 2010.
- Mendizabal, F.  
*Theoretical study of the interaction between Au(I) and I on the [AuI<sub>2</sub>](-)-I-2 complexes*  
Journal of Molecular Structure-Theochem, (955): 71-74 2010.
- Meng, Q.; Wang, F.; Li, M.  
*Bisoxazoline-copper(I)-catalyzed aziridination of diazoacetate with imines - A DFT study*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 981-990 2010.
- Menke, J. L.; Patterson, E. V.; McMahon, R. J.  
*Effects of Cyano Substituents on Cyclobutadiene and Its Isomers*  
Journal of Physical Chemistry A, (114): 6431-6437 2010.
- Mereau, R.; d'Antuono, P.; Castet, F.; Rouquet, G.; Robert, F.; Landais, Y.  
*Fragmentation of beta-Silyl Radicals. A Computational Study*  
Organometallics, (29): 2406-2412 2010.

Metzker, G.; Toledo, J. C., Jr.; Lima, F. C. A.; Magalhaes, A.; Cardoso, D. R.; Franco, D. W.  
*Nitric Oxide as an Activation Agent for Nucleophilic Attack in trans-[Ru(NO)(NH<sub>3</sub>)(4){P(OEt)<sub>3</sub>}](PF<sub>6</sub>)<sub>3</sub>*  
Journal of the Brazilian Chemical Society, (21): 1266-1273 2010.

Michalik, D.; Schulz, A.; Villinger, A.  
*Dichlorocyclodibismadiazane*  
Angewandte Chemie-International Edition, (49): 7575-7577 2010.

Michalik, S.; Machura, B.; Kruszynski, R.; Kusz, J.; Krompiec, M.  
*Synthesis, spectroscopic investigation, structural characterization and DFT calculation of the complexes [ReX<sub>2</sub>(N<sub>2</sub>COPh)(4-PhPyr)(PPh<sub>3</sub>)<sub>2</sub>] (X = Cl, Br)*  
Polyhedron, (29): 2629-2636 2010.

Mihaylov, T.; Trendafilova, N.; Georgieva, I.; Kostova, I.  
*Coordination properties of warfarin towards Pr(III) predicted from DFT and FT-IR studies*  
Chemical Physics, (374): 37-45 2010.

Milani, A.; Castiglioni, C.  
*Atomic charges from atomic polar tensors: A comparison of methods*  
Journal of Molecular Structure-Theochem, (955): 158-164 2010.

Milani, A.; Galimberti, D.; Castiglioni, C.; Zerbi, G.  
*Molecular charge distribution and charge fluxes from Atomic Polar Tensors: The case of OH bonds*  
Journal of Molecular Structure, (976): 342-349 2010.

Miller, K. L.; Williams, B. N.; Benitez, D.; Carver, C. T.; Ogilby, K. R.; Tkatchouk, E.; Goddard, W. A.; Diaconescu, P. L.  
*Dearomatization Reactions of N-Heterocycles Mediated by Group 3 Complexes*  
Journal of the American Chemical Society, (132): 342-355 2010.

Minisini, B.; Chavand, S.; Barthelery, R.; Tsobnang, F.  
*Calculations of the charge distribution in dodecyltrimethylammonium: a quantum chemical investigation*  
Journal of Molecular Modeling, (16): 1085-1092 2010.

Mitin, A. V.  
*Polarization of amino acids and their interaction in biomolecules*  
JETP Letters, (92): 360-364 2010.

Mitrasinovic, P. M.  
*Electronic Processes at Organic/Metal Interfaces: Recent Progress and Pitfalls*  
Current Organic Chemistry, (14): 198-211 2010.

Miyachi, H.; Matsui, T.; Shigeta, Y.; Yamashita, K.; Hirao, K.  
*Possibility of multi-conformational structure of mismatch DNA nucleobase in the presence of silver(I) ions*

Chemical Physics Letters, (495): 125-130 2010.

Mizuhata, Y.; Tokitoh, N.

*The first observation of (1)J(Sn-C) coupling constants in tin-carbon double-bond compounds*  
Applied Organometallic Chemistry, (24): 902-906 2010.

Mladek, A.; Sponer, J. E.; Jurecka, P.; Banas, P.; Otyepka, M.; Svozil, D.; Sponer, J.

*Conformational Energies of DNA Sugar-Phosphate Backbone: Reference QM Calculations and a Comparison with Density Functional Theory and Molecular Mechanics*  
Journal of Chemical Theory and Computation, (6): 3817-3835 2010.

Mo, Y.

*Computational evidence that hyperconjugative interactions are not responsible for the anomeric effect*  
Nature Chemistry, (2): 666-671 2010.

Mohajeri, A.; Shahamirian, M.

*The role of substituent on the aromaticity variation of mono- and di-substituted aza analogs of indole*  
Journal of Molecular Structure-Theochem, (951): 72-76 2010.

Mohajeri, A.; Shahamirian, M.

*Theoretical Study of Diels-Alder Reaction: Role of Substituent in Regioselectivity and Aromaticity*  
Journal of the Iranian Chemical Society, (7): 554-563 2010.

Mohamed, M. N. A.; Watts, H. D.; Guo, J.; Catchmark, J. M.; Kubicki, J. D.

*MP2, density functional theory, and molecular mechanical calculations of C-H center dot center dot center dot pi and hydrogen bond interactions in a cellulose-binding module-cellulose model system*  
Carbohydrate Research, (345): 1741-1751 2010.

Mohan, N.; Vijayalakshmi, K. P.; Koga, N.; Suresh, C. H.

*Comparison of Aromatic NH center dot center dot center dot pi, OH center dot center dot center dot pi, and CH center dot center dot center dot pi Interactions of Alanine Using MP2, CCSD, and DFT Methods*  
Journal of Computational Chemistry, (31): 2874-2882 2010.

Monajjemi, M.; Honaparvar, B.; Hadad, B. K.; Ilkhani, A. R.; Mollaamin, F.

*Thermo-chemical investigation and NBO analysis of some anxiolytic as Nano- drugs*  
African Journal of Pharmacy and Pharmacology, (4): 521-529 2010.

Monajjemi, M.; Lee, V. S.; Khaleghian, M.; Honaparvar, B.; Mollaamin, F.

*Theoretical Description of Electromagnetic Nonbonded Interactions of Radical, Cationic, and Anionic NH<sub>2</sub>BHNBHNH<sub>2</sub> Inside of the B18N18 Nanoring*  
Journal of Physical Chemistry C, (114): 15315-15330 2010.

Monakhov, K. Y.; Zessin, T.; Linti, G.

*Cubane-Like Bismuth-Iron Cluster: Synthesis, X-ray Crystal Structure and Theoretical Characterization of the [Bi<sub>4</sub>Fe<sub>8</sub>(CO)(28)](4-) Anion*  
European Journal of Inorganic Chemistry: 3212-3219 2010.

Monakhov, K. Y.; Zessin, T.; Linti, G.  
*Reduction vs. Metathesis in the Reactions of Bismuth Tribromide with a Bulky Lithium Silanide - An Experimental and Theoretical Study*  
European Journal of Inorganic Chemistry: 322-332 2010.

Monbaliu, J.-C.; Dive, G.; Marchand-Brynaert, J.; Peeters, D.  
*HDA cycloadditions of 1-diethoxyphosphonyl-1,3-butadiene with nitroso heterodienophiles: A computational investigation*  
Journal of Molecular Structure-Theochem, (959): 49-54 2010.

Montag, M.; Efremenko, I.; Cohen, R.; Shimon, L. J. W.; Leitus, G.; Diskin-Posner, Y.; Ben-David, Y.; Salem, H.; Martin, J. M. L.; Milstein, D.  
*Effect of CO on the Oxidative Addition of Arene C-H Bonds by Cationic Rhodium Complexes*  
Chemistry-a European Journal, (16): 328-353 2010.

Moran, M. D.; Brock, D. S.; Mercier, H. P. A.; Schrobilgen, G. J.  
*Xe<sub>3</sub>O<sub>3</sub><sup>+</sup>, a Precursor to a Noble-Gas Nitrate; Syntheses and Structural Characterizations of FXeONO<sub>2</sub>, XeF<sub>2</sub> center dot HNO<sub>3</sub>, and XeF<sub>2</sub> center dot N<sub>2</sub>O<sub>4</sub>*  
Journal of the American Chemical Society, (132): 13823-13839 2010.

Moss, R. A.; Zhang, M.; Krogh-Jespersen, K.  
*The Nucleophilic Reactivity of Fluoromethoxycarbene*  
Organic Letters, (12): 3476-3479 2010.

Muhammad, S.; Xu, H.; Janjua, M. R. S. A.; Su, Z.; Nadeem, M.  
*Quantum chemical study of benzimidazole derivatives to tune the second-order nonlinear optical molecular switching by proton abstraction*  
Physical Chemistry Chemical Physics, (12): 4791-4799 2010.

Mukherjee, A. J.; Zade, S. S.; Singh, H. B.; Sunoj, R. B.  
*Organoselenium Chemistry: Role of Intramolecular Interactions*  
Chemical Reviews, (110): 4357-4416 2010.

Mukhopadhyay, A.; Pandey, P.; Chakraborty, T.  
*Blue- and Red-Shifting CH center dot center dot center dot O Hydrogen Bonded Complexes between Haloforms and Ethers: Correlation of Donor nu(C-H) Spectral Shifts with C-O-C Angular Strain of the Acceptors*  
Journal of Physical Chemistry A, (114): 5026-5033 2010.

Muller, T.  
*Stability, Reactivity, and Strategies for the Synthesis of Silyliumylidenes, RSi:(+). A Computational Study*  
Organometallics, (29): 1277-1283 2010.

- Munha, R. F.; Antunes, M. A.; Alves, L. G.; Veiros, L. F.; Fryzuk, M. D.; Martins, A. M.  
*Structure and Reactivity of Neutral and Cationic trans-N,N'-Dibenzylcyclam Zirconium Alkyl Complexes*  
Organometallics, (29): 3753-3764 2010.
- Munz, D.; Strassner, T.  
*Mechanism and Regioselectivity of the Osmium-Catalyzed Aminohydroxylation of Olefins*  
Journal of Organic Chemistry, (75): 1491-1497 2010.
- Mutter, S. T.; Platts, J. A.  
*Modulation of Stacking Interactions by Transition-Metal Coordination: Ab Initio Benchmark Studies*  
Chemistry-a European Journal, (16): 5391-5399 2010.
- Nacereddine, A. K.; Yahia, W.; Bouacha, S.; Djerourou, A.  
*A theoretical investigation of the regio- and stereoselectivities of the 1,3-dipolar cycloaddition of C-diethoxyphosphoryl-N-methylnitron with substituted alkenes*  
Tetrahedron Letters, (51): 2617-2621 2010.
- Nadim, E. S.; Raissi, H.; Yoosefian, M.; Farzad, F.; Nowroozi, A. R.  
*Ab initio and DFT computational studies on molecular conformations and intramolecular hydrogen bonding in 3-mercaptop-but-2-enethial*  
Journal of Sulfur Chemistry, (31): 275-285 2010.
- Nahum, T. L.; Mamlok-Naaman, R.; Hofstein, A.; Taber, K. S.  
*Teaching and learning the concept of chemical bonding*  
Studies in Science Education, (46): 179-207 2010.
- Namura, K.; Kakuta, S.; Suzuki, H.  
*Synthesis of Ruthenium Polyhydride Clusters with 1,4,7-Triazacyclononane-Type Ligands: Stereo and Electronic Effects of Ancillary Ligands*  
Organometallics, (29): 4305-4311 2010.
- Nasertayoob, P.; Shahbazian, S.  
*Revisiting the Foundations of the Quantum Theory of Atoms in Molecules: The Subsystem Variational Procedure and the Finite Nuclear Models*  
International Journal of Quantum Chemistry, (110): 1188-1196 2010.
- Nasertayoob, P.; Shahbazian, S.  
*Revisiting the Foundations of the Quantum Theory of Atoms in Molecules: The Subsystem Variational Procedure and the Finite Nuclear Models*  
International Journal of Quantum Chemistry, (110): 1188-1196 2010.
- Nasiri, R.; Bahrami, H.; Zahedi, M.; Moosavi-Movahedi, A. A.; Sattarahmady, N.  
*A Theoretical Elucidation of Glucose Interaction with HSA's Domains*  
Journal of Biomolecular Structure and Dynamics, (28): 211-226 2010.
- Nazari, F.; Ansari, N.

*Theoretical insights into the trends in molecular properties of HCY, HSiY and HGeY molecules where Y = N, P, As*  
Journal of Molecular Modeling, (16): 1075-1084 2010.

Nazari, F.; Dorroodi, Z.  
*The Substitution Effect on Heavy Versions of Cyclobutadiene*  
International Journal of Quantum Chemistry, (110): 1514-1528 2010.

Ndassa, I. M.; Silvi, B.; Volatron, F.  
*Understanding Reaction Mechanisms in Organic Chemistry from Catastrophe Theory: Ozone Addition on Benzene*  
Journal of Physical Chemistry A, (114): 12900-12906 2010.

Neela, Y. I.; Mahadevi, A. S.; Sastry, G. N.  
*Hydrogen Bonding in Water Clusters and Their Ionized Counterparts*  
Journal of Physical Chemistry B, (114): 17162-17171 2010.

Neil, S. R. T.; Evans, C. J.  
*Computational study on the energies and structures of the [H, Si, N, C, S] isomers*  
Theoretical Chemistry Accounts, (127): 661-669 2010.

Nemeth, B.; Khater, B.; Guillemin, J.-C.; Veszpremi, T.  
*Differences Between Amine- and Phosphine-Boranes: Synthesis, Photoelectron Spectroscopy, and Quantum Chemical Study of the Cyclopropylidic Derivatives*  
Inorganic Chemistry, (49): 4854-4864 2010.

Neugebauer, J.  
*Chromophore-specific theoretical spectroscopy: From subsystem density functional theory to mode-specific vibrational spectroscopy*  
Physics Reports-Review Section of Physics Letters, (489): 1-87 2010.

Nguyen Tien, T.; Tran Thanh, H.; Minh Tho, N.  
*Theoretical analysis of the (HNO)(2), (HNO center dot center dot center dot HNS), and (HNS)(2) dimers - A case of red and blue shifts of N-H stretching frequency*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 849-857 2010.

Nguyen, T. T.; Tran, T. H.; Minh, T. N.  
*Theoretical analysis of the (HNO)(2), (HNO center dot center dot center dot HNS), and (HNS)(2) dimers - A case of red and blue shifts of N-H stretching frequency*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 849-857 2010.

Nicolas-Vazquez, I.; Mendez-Albores, A.; Moreno-Martinez, E.; Miranda, R.; Castro, M.  
*Role of Lactone Ring in Structural, Electronic, and Reactivity Properties of Aflatoxin B1: A Theoretical Study*  
Archives of Environmental Contamination and Toxicology, (59): 393-406 2010.

Niu, Y.; Feng, S.; Ding, Y.; Qu, R.; Wang, D.; Han, J.  
*Theoretical Investigation on Sulfur-Containing Chelating Resin-Divalent Metal Complexes*

International Journal of Quantum Chemistry, (110): 1982-1993 2010.

Nockemann, P.; Pellens, M.; Van Hecke, K.; Van Meervelt, L.; Wouters, J.; Thijs, B.; Vanecht, E.; Parac-Vogt, T. N.; Mehdi, H.; Schaltin, S.; Fransaer, J.; Zahn, S.; Kirchner, B.; Binnemans, K.

*Cobalt(II) Complexes of Nitrile-Functionalized Ionic Liquids*

Chemistry-a European Journal, (16): 1849-1858 2010.

Nori-Shargh, D.; Hassanzadeh, N.; Kosari, M.; Rabiekarahroudi, P.; Yahyaei, H.; Sharifi, S.

*Stereoelectronic interaction effects on the conformational properties of 5-methyl-5-aza-1,3-dithiacyclohexane and its analogous containing N, P, O, and Se atoms - A hybrid density functional theory (DFT), ab initio study, and natural bond orbital (NBO) analysis*

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 579-587 2010.

Nori-Shargh, D.; Khamooshi-Sarabi, A.; Sharifi, S.; Sheikh-Ansari, E.

*Hybrid-DFT Study and NBO Analysis of the Stereoelectronic Interaction Effects (Associated with the Anomeric Effects) on the Conformational Properties of 2,3,5,6-Tetrahalo-1,4-dioxanes and Their Analogs Containing S and Se Atoms*

Phosphorus Sulfur and Silicon and the Related Elements, (185): 2122-2134 2010.

Nori-Shargh, D.; Yahyaei, H.; Boggs, J. E.

*Stereoelectronic interaction effects on the conformational properties of hydrogen peroxide and its analogues containing S and Se atoms: An ab initio, hybrid-DFT study and NBO analysis*

Journal of Molecular Graphics and Modelling, (28): 807-813 2010.

Norrby, P.-O.; Petersen, T. B.; Bielawski, M.; Olofsson, B.

*alpha-Arylation by Rearrangement: On the Reaction of Enolates with Diaryliodonium Salts*

Chemistry-a European Journal, (16): 8251-8254 2010.

Nunes, S. C. C.; Lopes Jesus, A. J.; Joao Moreno, M.; Eusebio, M. E. S.

*Conformational preferences of alpha,alpha-trehalose in gas phase and aqueous solution*

Carbohydrate Research, (345): 2048-2059 2010.

Nycz, J. E.; Malecki, G.; Morag, M.; Nowak, G.; Ponikiewski, L.; Kusz, J.; Switlicka, A.

*Arbutin: Isolation, X-ray structure and computational studies*

Journal of Molecular Structure, (980): 13-17 2010.

Olah, G. A.; Prakash, G. K. S.; Rasul, G.

*Vicinal dihalonium ions: diprotonated and dimethylated chlorine [H<sub>2</sub>Cl<sub>2</sub>2+, (CH<sub>3</sub>)<sub>2</sub>Cl-2(2+)] and bromine [H<sub>2</sub>Br<sub>2</sub>2+, (CH<sub>3</sub>)<sub>2</sub>Br-2(2+)] dication*

Proceedings of the National Academy of Sciences of the United States of America, (107): 6716-6720 2010.

Oliaey, A. R.; Boshra, A.; Khavary, M.

*Spin polarized bonding analysis of endohedral boron nitride nanocages: Density functional theory study*

Physica E-Low-Dimensional Systems & Nanostructures, (42): 2314-2318 2010.

Oliva, J. M.; Fernandez-Barbero, A.; Serrano-Andres, L.; Canle-L, M.; Arturo Santaballa, J.; Isabel Fernandez, M.

*Energy landscapes in diexo and exo/endo isomers derived from Li<sub>2</sub>B<sub>12</sub>H<sub>12</sub>*  
Chemical Physics Letters, (497): 172-177 2010.

Ortega-Moo, C.; Cervantes, J.; Angel Mendez-Rojas, M.; Pannell, K. H.; Merino, G.

*What is the structure of Si<sub>3</sub>H<sub>5</sub>-?*  
Chemical Physics Letters, (490): 1-3 2010.

Ou, P.; Shen, W.; Xie, X.; Zeng, C.; Li, M.

*Density functional theory investigation on the electronic structure of furo[3,4-*b*]pyridine-type heterocyclics: from monomer to polymer*  
Structural Chemistry, (21): 1253-1261 2010.

Oziminski, W. P.; Krygowski, T. M.

*Natural bond orbital (NBO) analysis of the angular group induced bond alternation (AGIBA) substituent effect*  
Journal of Physical Organic Chemistry, (23): 551-556 2010.

Oziminski, W. P.; Krygowski, T. M.; Fowler, P. W.; Soncini, A.

*Aromatization of Fulvene by Complexation with Lithium*  
Organic Letters, (12): 4880-4883 2010.

Padilla-Campos, L.; Chavez, E.

*Electronic properties of small K-n (n <= 8) and bimetallic KnCum (n, m <= 4) clusters*  
Journal of Molecular Structure-Theochem, (958): 92-100 2010.

Pakiari, A. H.; Azami, S. M.

*Hyperconjugation versus back bonding in AH(3-n)X(n) species (A = Si and Ge; X = F, Cl and Br; and n=1, 2 and 3)*  
Journal of Molecular Structure-Theochem, (939): 65-68 2010.

Pakiari, A. H.; Farrokhnia, M.

*Theoretical Study of Heteroatom Resonance-Assisted Hydrogen Bond: Effect of Substituent on pi-delocalization*  
Iranian Journal of Chemistry & Chemical Engineering-International English Edition, (29): 197-210  
2010.

Pakiari, A. H.; Jamshidi, Z.

*Nature and Strength of M-S Bonds (M = Au, Ag, and Cu) in Binary Alloy Gold Clusters*  
Journal of Physical Chemistry A, (114): 9212-9221 2010.

Pakiari, A. H.; Mousavi, M.

*A Detailed Study of the Electronic Structure of Fe-3 Cluster and Associative Adsorption of N-2 to This Cluster: A Natural Bond Orbital Analysis*  
Journal of Physical Chemistry A, (114): 10209-10216 2010.

Pakiari, A. H.; Mousavi, M.

*A Detailed Study of the Electronic Structure of Fe-3 Cluster and Associative Adsorption of N-2 to This Cluster: A Natural Bond Orbital Analysis*  
Journal of Physical Chemistry A, (114): 10209-10216 2010.

Pakiari, A. H.; Siahrostami, S.; Ziegler, T.  
*An insight into microscopic properties of aprotic ionic liquids: A DFT study*  
Journal of Molecular Structure-Theochem, (955): 47-52 2010.

Palmer, D. S.; Sergiievskyi, V. P.; Jensen, F.; Fedorov, M. V.  
*Accurate calculations of the hydration free energies of druglike molecules using the reference interaction site model*  
Journal of Chemical Physics, (133) 2010.

Panda, M. K.; Shaikh, M. M.; Ghosh, P.  
*Controlled oxidation of organic sulfides to sulfoxides under ambient conditions by a series of titanium isopropoxide complexes using environmentally benign H2O2 as an oxidant*  
Dalton Transactions, (39): 2428-2440 2010.

Pandey, K. K.; Lledos, A.  
*Linear versus bent bonding in metal-phosphinidene complexes: Theoretical studies of the electrophilic phosphinidene complexes  $[(Cp)(CO)(2)M\text{PMe}]^+$ ,  $[(Cp)(CO)(3)M=\text{PMe}]^+ (M = Cr, Mo, W)$*   
Journal of Organometallic Chemistry, (695): 206-214 2010.

Pandey, K. K.; Patidar, P.; Aldridge, S.  
*Nature of M-Ga Bonds in Dihalogallyl Complexes  $(\eta_5\text{-C}_5\text{H}_5)(\text{Me}_3\text{P})(2)\text{M}(\text{GaX}_2)$  ( $\text{M} = \text{Fe}, \text{Ru}, \text{Os}$ ) and  $(\eta_5\text{-C}_5\text{H}_5)(\text{OC})(2)\text{Fe}(\text{GaX}_2)$  ( $X = \text{Cl}, \text{Br}, \text{I}$ ): A DFT Study*  
Journal of Physical Chemistry A, (114): 12099-12105 2010.

Pandey, K. K.; Patidar, P.; Braunschweig, H.  
*Structure and Bonding Energy Analysis of M-Ga Bonds in Dihalogallyl Complexes  $trans-[X(\text{PMe}_3)(2)\text{M}(\text{GaX}_2)]$  ( $\text{M} = \text{Ni}, \text{Pd}, \text{Pt}; X = \text{Cl}, \text{Br}, \text{I}$ )*  
Inorganic Chemistry, (49): 6994-7000 2010.

Papanikolaou, P.; Karafiloglou, P.  
*Investigating sigma bonds in an electric field from the Pauling's perspective: the behavior of Cl-X and H-X ( $X = \text{C}, \text{Si}$ ) bonds*  
Theoretical Chemistry Accounts, (126): 213-222 2010.

Parameswaran, P.; Frenking, G.  
*Chemical Bonding in Transition Metal Complexes with Beryllium Ligands  $[(\text{PMe}_3)(2)\text{M-BeCl}_2]$ ,  $[(\text{PMe}_3)(2)\text{M-BeClMe}]$ , and  $[(\text{PMe}_3)(2)\text{M-BeMe}_2]$  ( $\text{M} = \text{Ni}, \text{Pd}, \text{Pt}$ )*  
Journal of Physical Chemistry A, (114): 8529-8535 2010.

Pardo, E.; Ferrando-Soria, J.; Dul, M.-C.; Lescouezec, R.; Journaux, Y.; Ruiz-Garcia, R.; Cano, J.; Julve, M.; Lloret, F.; Canadillas-Delgado, L.; Pasan, J.; Ruiz-Perez, C.  
*Oligo-m-phenyleneoxalamide Copper(II) Mesocates as Electro-Switchable Ferromagnetic Metal-Organic Wires*

Chemistry-a European Journal, (16): 12838-12851 2010.

Partal Urena, F.; Aviles Moreno, J. R.; Lopez Gonzalez, J. J.

*Rotational Strength Sign and Normal Modes Description: A Theoretical and Experimental Comparative Study in Bicyclic Terpenes*  
Chirality, (22): E123-E129 2010.

Parveen, S.; Chandra, A. K.; Zeegers-Huyskens, T.

*Theoretical investigation of the hydrogen bonding interaction between substituted phenols and simple O- and N-bases*  
Journal of Molecular Structure, (977): 258-265 2010.

Pascual, S.; Blin, T.; Saikia, P. J.; Thomas, M.; Gosselin, P.; Fontaine, L.

*Block Copolymers Based on 2-Vinyl-4,4-dimethyl-5-oxazolone by RAFT Polymerization: Experimental and Computational Studies*  
Journal of Polymer Science Part a-Polymer Chemistry, (48): 5053-5062 2010.

Pathak, S.; Kumar, A.; Tandon, P.

*Molecular structure and vibrational spectroscopic investigation of 4-chloro-4' dimethylamino-benzylidene aniline using density functional theory*  
Journal of Molecular Structure, (981): 1-9 2010.

Pathmalingam, T.; Habib, F.; Widdifield, C. M.; Loiseau, F.; Burchell, T. J.; Gorelsky, S. I.; Beauchemin, A. M.; Bryce, D. L.; Murugesu, M.

*Combining oximes with azides to create a novel 1-D [NaCo2III] system: synthesis, structure and solid-state NMR*  
Dalton Transactions, (39): 1504-1510 2010.

Patil, M. P.; Sharma, A. K.; Sunoj, R. B.

*Importance of the Nature of alpha-Substituents in Pyrrolidine Organocatalysts in Asymmetric Michael Additions*  
Journal of Organic Chemistry, (75): 7310-7321 2010.

Patroniak, V.; Markiewicz, P. L.; Hoffmann, M.

*Quantum chemical studies on chameleonic ligand and its grid-type copper(I) and zinc(II) complexes*  
Journal of Molecular Structure-Theochem, (949): 82-87 2010.

Payaka, A.; Tongraar, A.; Rode, B. M.

*QM/MM Dynamics of CH<sub>3</sub>COO-Water Hydrogen Bonds in Aqueous Solution*  
Journal of Physical Chemistry A, (114): 10443-10453 2010.

Peles-Lemli, B.; Matisz, G.; Kelterer, A.-M.; Fabian, W. M. F.; Kunsagi-Mate, S.

*Noncovalent Interaction between Aniline and Carbon Nanotubes: Effect of Nanotube Diameter and the Hydrogen-Bonded Solvent Methanol on the Adsorption Energy and the Photophysics*  
Journal of Physical Chemistry C, (114): 5898-5905 2010.

Peng, X.; Cui, G.-h.; Li, D.-j.; Liu, T.-f.

*Synthesis, characterization, and theoretical calculations of mononuclear copper(II) benzoate complex with 2-propylimidazole, [Cu(PIM)(2)(PhCOO)(2)]*  
Journal of Molecular Structure, (967): 54-60 2010.

Peng, X.; Cui, G.-H.; Li, D.-J.; Wu, S.-Z.; Yu, Y.-M.  
*Structure, spectroscopy, and theory calculations of mononuclear mixed-ligand copper(II) complex with malonate and 2-propylimidazole, [Cu(mal)(PIM)(2)(H<sub>2</sub>O)]*  
Journal of Molecular Structure, (971): 47-52 2010.

Perez-Badell, Y.; Solans-Monfort, X.; Sodupe, M.; Montero, L. A.  
*A DFT periodic study on the interaction between O-2 and cation exchanged chabazite MCHA (M = H<sup>+</sup>, Na<sup>+</sup> or Cu<sup>+</sup>): effects in the triplet-singlet energy gap*  
Physical Chemistry Chemical Physics, (12): 442-452 2010.

Perez-Galan, P.; Delpont, N.; Herrero-Gomez, E.; Maseras, F.; Echavarren, A. M.  
*Metal-Arene Interactions in Dialkylbiarylphosphane Complexes of Copper, Silver, and Gold*  
Chemistry-a European Journal, (16): 5324-5332 2010.

Perrin, L.; Kirillov, E.; Carpentier, J.-F.; Maron, L.  
*DFT Investigation of the Tacticity Control during Styrene Polymerization Catalyzed by Single-Component Allyl ansa-Lanthanidocenes {(C<sub>5</sub>H<sub>4</sub>CMe<sub>2</sub>(9-C<sub>13</sub>H<sub>8</sub>)}Ln(C<sub>3</sub>H<sub>5</sub>)}*  
Macromolecules, (43): 6330-6336 2010.

Petz, W.; Neumueller, B.; Tonner, R.  
*Reaction of Double Ylide C(PPh<sub>3</sub>)(2) with [W(CO)(6)] - Crystal Structures of [(CO)(5)W(CCPPh<sub>3</sub>)] and [(CO)(5)W{eta}(1)-O<sub>2</sub>C<sub>2</sub>(PPh<sub>3</sub>)(2)] and Bonding Analyses of [TM(CCPPh<sub>3</sub>)] Compounds*  
European Journal of Inorganic Chemistry: 1872-1880 2010.

Pfirrmann, S.; Limberg, C.; Herwig, C.; Knispel, C.; Braun, B.; Bill, E.; Stoesser, R.  
*A Reduced beta-Diketiminato-Ligated Ni<sub>3</sub>H<sub>4</sub> Unit Catalyzing H/D Exchange*  
Journal of the American Chemical Society, (132): 13684-13691 2010.

Pham Ngoc, D.; Hue Minh Thi, N.; Tran Thanh, H.; Zeegers-Huyskens, T.  
*Theoretical investigation of the interaction between monohalogenated ethenes and hydrogen peroxide*  
Journal of Molecular Structure, (976): 73-80 2010.

Philips, J. J.; Hudspeth, M. A.; Browne, P. M., Jr.; Peralta, J. E.  
*Basis set dependence of atomic spin populations*  
Chemical Physics Letters, (495): 146-150 2010.

Phukan, A. K.; Guha, A. K.  
*Nature of Transannular Intramolecular Interactions in Group 4 and 6 Metallatranes: A Combined Density Functional Theory and Atoms in Molecules Theory Study*  
Inorganic Chemistry, (49): 9884-9890 2010.

Phukan, A. K.; Guha, A. K.; Silvi, B.  
*Is delocalization a prerequisite for stability of ring systems? A case study of some inorganic rings*

Dalton Transactions, (39): 4126-4137 2010.

Picot, D.; Ohanessian, G.; Frison, G.

*Thermodynamic Stability Versus Kinetic Lability of ZnS4 Core*  
Chemistry-an Asian Journal, (5): 1445-1454 2010.

Pilz, T. D.; Rockstroh, N.; Rau, S.

*Synthesis and characterization of heterooligonuclear ruthenium complexes with tri(phenanthrolino)hexaazatriphenylene ligands*  
Journal of Coordination Chemistry, (63): 2727-2742 2010.

Piperno, A.; Giofre, S. V.; Iannazzo, D.; Romeo, R.; Romeo, G.; Chiacchio, U.; Rescifina, A.; Piotrowska, D. G.

*Synthesis of C-4' Truncated Phosphonated Carbocyclic 2'-Oxa-3'-azanucleosides as Antiviral Agents*  
Journal of Organic Chemistry, (75): 2798-2805 2010.

Plutecka, A.; Rychlewska, U.; Prusinowska, N.; Gawronski, J.

*Solid solution of two diastereomers of [3aR,S],7a(R,S)]-3-[(1'R)-1-phenylethyl]perhydro-1,3-benzothiazol-2-iminium chloride*  
Acta Crystallographica Section B-Structural Science, (66): 678-686 2010.

Podlech, J.

*Stereoelectronic Effects in alpha-Carbonions of Conformationally Constrained Sulfides, Sulfoxides, and Sulfones*  
Journal of Physical Chemistry A, (114): 8480-8487 2010.

Popp, B. V.; Morales, C. M.; Landis, C. R.; Stahl, S. S.

*Electronic Structural Comparison of the Reactions of Dioxygen and Alkenes with Nitrogen-Chelated Palladium(0)*  
Inorganic Chemistry, (49): 8200-8207 2010.

Postigo, L.; Bellarosa, L.; Sanchez-Nieves, J.; Royo, P.; Lledos, A.; Mosquera, M. E. G.

*Dinuclear Dicyclopentadienyl Titanium Complexes with Bridging Cyclopentadienylsiloxo Ligands*  
Organometallics, (29): 642-655 2010.

Powers, D. C.; Benitez, D.; Tkatchouk, E.; Goddard, W. A., III; Ritter, T.

*Bimetallic Reductive Elimination from Dinuclear Pd(III) Complexes*  
Journal of the American Chemical Society, (132): 14092-14103 2010.

Pradhan, K.; Gutsev, G. L.; Jena, P.

*Negative ions of transition metal-halogen clusters*  
Journal of Chemical Physics, (133) 2010.

Pratihar, S.; Roy, S.

*Nucleophilicity and Site Selectivity of Commonly Used Arenes and Heteroarenes*  
Journal of Organic Chemistry, (75): 4957-4963 2010.

Prestianni, A.; Joubert, L.; Chagnes, A.; Cote, G.; Ohnet, M.-N.; Rabbe, C.; Charbonnel, M.-C.; Adamo, C.  
*IR Fingerprints of U(VI) Nitrate Monoamides Complexes: A Joint Experimental and Theoretical Study*  
Journal of Physical Chemistry A, (114): 10878-10884 2010.

Pu, L.; Sun, Y.; Zhang, Z.  
*Hydrogen Bonding in Hydrates with one Acetic Acid Molecule*  
Journal of Physical Chemistry A, (114): 10842-10849 2010.

Pu, Z.; Ge, M.; Li, Q.  
*MB82- (M = Be, Mg, Ca, Sr, and Ba): Planar octacoordinate alkaline earth metal atoms enclosed by boron rings*  
Science China-Chemistry, (53): 1737-1745 2010.

Qi, D.; Zhang, Y.; Zhang, L.; Jiang, J.  
*Structures and Spectroscopic Properties of Fluoroboron-Subtriazaporphyrin Derivatives: Density Functional Theory Approach on the Benzo-Fusing Effect*  
Journal of Physical Chemistry A, (114): 1931-1938 2010.

Qi, Q.; Ha, Y.; Sun, Y.  
*Density functional studies of the substituent effect on absorption and emission properties of 1, 8-naphthalimide derivatives*  
Journal of Molecular Modeling, (16): 1179-1186 2010.

Qi, Y.; Mu, Z.; Zhang, Y.; Feng, D.  
*Insertion reactions of the p-complex structure of silylenoid into C-X bonds (X = F, Cl, Br, O, and N)*  
Structural Chemistry, (21): 879-884 2010.

Qi, Y.; Mu, Z.; Zhang, Y.; Feng, D.  
*The isomeric structures and stability of pentacoordinate silylenoid PhCH<sub>2</sub>(OH)CH<sub>3</sub>SiLiF*  
Journal of Molecular Structure-Theochem, (953): 49-54 2010.

Qian, Z.; Feng, H.; Yang, W.; Jin, X.; Wang, Y.; Bi, S.  
*Density functional studies of the structural characteristics, Al-27 NMR chemical shifts and water-exchange reactions of Al<sub>3</sub>O<sub>8</sub>(OH)(56)(H<sub>2</sub>O)(26)(18+)(Al-30) in aqueous solution*  
Geochimica et Cosmochimica Acta, (74): 1230-1237 2010.

Qin, H.; Li, Z.-F.  
*Theoretical Study of the Hydrogen Bond Character between the Fno and Ho2 Radical*  
Journal of Theoretical & Computational Chemistry, (9): 925-934 2010.

Quintero, L.; Sanchez-Vazquez, M.; Cruz-Gregorio, S.; Sartillo-Piscil, F.  
*On the Existence of the Chair Conformation in Six-Membered Ring Phosphates Bearing an Aryl Group Axially Oriented at the C4 Position: Cyclic Nucleotides As Model Compounds for Cyclic Phosph(on)ate and Phosphoramido Prodrugs*  
Journal of Organic Chemistry, (75): 5852-5859 2010.

Rabilloud, F.

*Structure and Electronic Properties of Alkali-C-60 Nanoclusters*  
Journal of Physical Chemistry A, (114): 7241-7247 2010.

Raiissi, H.; Jalbout, A. F.; Abbasi, B.; Fazli, F.; Farzad, F.; Nadim, E.; De Leon, A.  
*Intramolecular Hydrogen Bond in 3-Imino-Propenylamine Isomers: AIM and NBO Studies*  
International Journal of Quantum Chemistry, (110): 893-901 2010.

Raiissi, H.; Jalbout, A. F.; Yoosefian, M.; Fazli, M.; Nowroozi, A.; Shahinin, M.; De Leon, A.  
*Intramolecular Hydrogen Bonding in Structural Conformers of 2-Amino Methylenemalonaldehyde: AIM and NBO Studies*  
International Journal of Quantum Chemistry, (110): 821-830 2010.

Ramasami, K.; Ramalingam, M.; Venuvanalingam, P.; Jaccob, M.  
*Singlet Methylenne Insertion Into Polar O-H and N-H Bonds of Water and Ammonia-Ab Initio and DFT Study*  
International Journal of Quantum Chemistry, (110): 1310-1316 2010.

Ramasami, P.; Ford, T. A.  
*Ab initio studies of the vibrational spectra of some hydrogen-bonded complexes of fluoroacetylene*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 716-724 2010.

Ramos, L. A.; Ulic, S. E.; Romano, R. M.; Erben, M. F.; Lehmann, C. W.; Bernhardt, E.; Beckers, H.; Willner, H.; Della Vedova, C. O.  
*Vibrational Spectra, Crystal Structures, Constitutional and Rotational Isomerism of FC(O)SCN and FC(O)NCS*  
Inorganic Chemistry, (49): 11142-11157 2010.

Raschi, A. B.; Romano, E.; Benavente, A. M.; Ben Altabef, A.; Tuttolomondo, M. E.  
*Structural and vibrational analysis of thymoquinone*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (77): 497-505 2010.

Ravi, P.; Gore, G. M.; Venkatesan, V.; Tewari, S. P.; Sikder, A. K.  
*Theoretical studies on the structure and detonation properties of amino-, methyl-, and nitro-substituted 3,4,5-trinitro-1H-pyrazoles*  
Journal of Hazardous materials, (183): 859-865 2010.

Ravikumar, C.; Joe, I. H.  
*Electronic absorption and vibrational spectra and nonlinear optical properties of 4-methoxy-2-nitroaniline*  
Physical Chemistry Chemical Physics, (12): 9452-9460 2010.

Ravikumar, C.; Joe, I. H.; Sajan, D.  
*Vibrational contributions to the second-order nonlinear optical properties of pi-conjugated structure acetoacetanilide*  
Chemical Physics, (369): 1-7 2010.

Rayon, V. M.; Barrientos, C.; Redondo, P.; Largo, A.

*A computational study of arsenic dicarbide (C<sub>2</sub>As)*  
Chemical Physics Letters, (485): 286-289 2010.

Rhyman, L.; Abdallah, H. H.; Jhaumeer-Laulloo, S.; Domingo, L. R.; Joule, J. A.; Ramasami, P.  
*The 1,3-dipolar cycloaddition of 1H-pyridinium-3-olate and 1-methylpyridinium-3-olate with methyl acrylate a density functional theory study*  
Tetrahedron, (66): 9187-9193 2010.

Rhyman, L.; Abdallah, H. H.; Ramasami, P.  
*Quantum mechanical study of the structure and spectroscopic characterisation of the novel trisilylsilylcyanide and trigermethylgermethylcyanide in the gas phase*  
Polyhedron, (29): 1168-1174 2010.

Ribas, X.; Calle, C.; Poater, A.; Casitas, A.; Gomez, L.; Xifra, R.; Parella, T.; Benet-Buchholz, J.; Schweiger, A.; Mitrikas, G.; Sola, M.; Llobet, A.; Stack, T. D. P.  
*Facile C-H Bond Cleavage via a Proton-Coupled Electron Transfer Involving a C-H center dot center dot center dot Cu-II Interaction*  
Journal of the American Chemical Society, (132): 12299-12306 2010.

Ribeiro da Silva, M. A. V.; Ribeiro da Silva, M. d. D. M. C.; Santos, A. F. L. O. M.; Roux, M. V.; Foces-Foces, C.; Notario, R.; Guzman-Mejia, R.; Juaristi, E.  
*Experimental and Computational Thermochemical Study of alpha-Alanine (DL) and beta-Alanine*  
Journal of Physical Chemistry B, (114): 16471-16480 2010.

Rigamonti, L.; Forni, A.; Manassero, M.; Manassero, C.; Pasini, A.  
*Cooperation between Cis and Trans Influences in cis-Pt-II(PPh<sub>3</sub>)<sub>2</sub> Complexes: Structural, Spectroscopic, and Computational Studies*  
Inorganic Chemistry, (49): 123-135 2010.

Rimarcik, J.; Lukes, V.; Klein, E.; Ilcin, M.  
*Study of the solvent effect on the enthalpies of homolytic and heterolytic N-H bond cleavage in p-phenylenediamine and tetracyano-p-phenylenediamine*  
Journal of Molecular Structure-Theochem, (952): 25-30 2010.

Rios-Font, R.; Sodupe, M.; Rodriguez-Santiago, L.; Taylor, P. R.  
*The Role of Exact Exchange in the Description of Cu<sup>2+</sup>-(H<sub>2</sub>O)<sub>(n)</sub> (n=1-6) Complexes by Means of DFT Methods*  
Journal of Physical Chemistry A, (114): 10857-10863 2010.

Roble, N. L.; Cutin, E. H.; Mews, R.; Della Vedova, C. O.  
*Pentafluoroethylminosulfur difluoride, CF<sub>3</sub>CF<sub>2</sub>N-SF<sub>2</sub>: Vibrational spectra and quantum chemical calculations*  
Journal of Molecular Structure, (978): 131-135 2010.

Roohi, H.; Akbari, F.  
*Adsorption of parent nitrosamine on the nanocrystalline H-zeolite: A theoretical study*  
Applied Surface Science, (256): 7575-7582 2010.

- Roohi, H.; Nowroozi, A.; Bavafa, S.; Akbary, F.; Eshghi, F.  
*Interaction Between NH<sub>2</sub>NO and H<sub>2</sub>O<sub>2</sub>: A Quantum Chemistry Study*  
International Journal of Quantum Chemistry, (110): 1972-1981 2010.
- Roohi, H.; Nowroozi, A.-r.; Ebrahimi, A.; Makiabadi, B.  
*Effect of CH<sub>3</sub>CO functional group on the molecular and electronic properties of BN43zz nanotube: A computational chemistry study*  
Journal of Molecular Structure-Theochem, (952): 36-45 2010.
- Roohi, H.; Nowroozi, A.-R.; Eshghi, F.  
*The Gas Phase Hydrogen-Bonded Dimers of HOCl: A High-Level Quantum Chemical Study*  
International Journal of Quantum Chemistry, (110): 1489-1499 2010.
- Roos, G.; Geerlings, P.; Messens, J.  
*The conserved active site tryptophan of thioredoxin has no effect on its redox properties*  
Protein Science, (19): 190-194 2010.
- Rosas, F.; Dominguez, R. M.; Mora, J. R.; Marquez, E.; Cordova, T.; Chuchani, G.  
*Combined experimental and theoretical studies of the elimination kinetic of 2-methoxytetrahydropyran in the gas phase*  
Journal of Physical Organic Chemistry, (23): 1127-1136 2010.
- Rosas, F.; Dominguez, R. M.; Tosta, M.; Mora, J. R.; Marquez, E.; Cordova, T.; Chuchani, G.  
*The mechanism of the homogeneous, unimolecular gas-phase elimination kinetic of 1,1-dimethoxycyclohexane: experimental and theoretical studies*  
Journal of Physical Organic Chemistry, (23): 743-750 2010.
- Rougier, L.; Milon, A.; Reat, V.; Jolibois, F.  
*Modelling the influence of hydrogen bond network on chemical shielding tensors description. GIAO-DFT study of WALP23 transmembrane alpha-helix as a test case*  
Physical Chemistry Chemical Physics, (12): 6999-7008 2010.
- Roux, M. V.; Foces-Foces, C.; Notario, R.; Ribeiro da Silva, M. A. V.; Ribeiro da Silva, M. d. D. M. C.; Santos, A. F. L. O. M.; Juaristi, E.  
*Experimental and Computational Thermochemical Study of Sulfur-Containing Amino Acids: L-Cysteine, L-Cystine, and L-Cysteine-Derived Radicals. S-S, S-H, and C-S Bond Dissociation Enthalpies*  
Journal of Physical Chemistry B, (114): 10530-10540 2010.
- Roux, M. V.; Notario, R.; Foces-Foces, C.; Temprado, M.; Ros, F.; Emel'yanenko, V. N.; Verevkin, S. P.  
*Experimental and Computational Thermochemical Study and Solid-Phase Structure of 5,5-Dimethylbarbituric Acid*  
Journal of Physical Chemistry A, (114): 3583-3590 2010.
- Roux, M. V.; Temprado, M.; Jimenez, P.; Foces-Foces, C.; Notario, R.; Parameswar, A. R.; Demchenko, A. V.; Chickos, J. S.; Deakyne, C. A.; Liebman, J. F.  
*Experimental and Theoretical Study of the Structures and Enthalpies of Formation of 3H-1,3-Benzoxazole-2-thione, 3H-1,3-Benzothiazole-2-thione, and Their Tautomers*

Journal of Physical Chemistry A, (114): 6336-6341 2010.

Roy, D.; Sunoj, R. B.

*Ni-, Pd-, or Pt-catalyzed ethylene dimerization: a mechanistic description of the catalytic cycle and the active species*

Organic & Biomolecular Chemistry, (8): 1040-1051 2010.

Ruette, F.; Sanchez, M.; Castellano, O.; Soscun, H.

*Methodologies to Analyze Surface Bonding Properties Using Parametric and Density Functional Methods*

International Journal of Quantum Chemistry, (110): 743-754 2010.

Safi, Z. S.; Lamsabhi, A. M.

*A theoretical density functional study of association of Zn<sup>2+</sup> with oxazolidine and its thio derivatives in the gas phase*

Journal of Physical Organic Chemistry, (23): 751-758 2010.

Saikin, S. K.; Chu, Y.; Rappoport, D.; Crozier, K. B.; Aspuru-Guzik, A.

*Separation of Electromagnetic and Chemical Contributions to Surface-Enhanced Raman Spectra on Nanoengineered Plasmonic Substrates*

Journal of Physical Chemistry Letters, (1): 2740-2746 2010.

Sajan, D.; Erdogan, Y.; Kuruvilla, T.; Joe, I. H.

*Vibrational spectra and first-order molecular hyperpolarizabilities of p-hydroxybenzaldehyde dimer*

Journal of Molecular Structure, (983): 12-21 2010.

Salamanca M, C.; Tiznado V, W.; Jaramillo G, P.

*Experimental and Theoretical Study of Shynthesis of N-Alkyl-Nitroimidazoles*

Vitae-Revista De La Facultad De Quimica Farmaceutica, (17): 199-208 2010.

Salavati-Niasari, M.; Mirsattari, S. N.; Monajjemi, M.; Hamadanian, M.

*Density functional B3LYP and B3PW91 studies of the properties of four cyclic organodiboranes with tetramethylene fragments*

Journal of Structural Chemistry, (51): 437-443 2010.

Saloni, J.; Dasary, S. S. R.; Anjaneyulu, Y.; Yu, H.; Hill, G., Jr.

*Molecularly imprinted polymers for detection of explosives: computational study on molecular interactions of 2,6-dinitrotoluene and methacrylic acid complex*

Structural Chemistry, (21): 1171-1184 2010.

Saloni, J.; Kolodziejczyk, W.; Roszak, S.; Majumdar, D.; Hill, G., Jr.; Leszczynski, J.

*Local and Global Electronic Effects in Single and Double Boron-Doped Carbon Nanotubes*

Journal of Physical Chemistry C, (114): 1528-1533 2010.

Samanta, A. K.; Pandey, P.; Bandyopadhyay, B.; Chakraborty, T.

*Cooperative Strengthening of an Intramolecular O-H center dot center dot center dot O Hydrogen Bond by a Weak C-H center dot center dot center dot O Counterpart: Matrix-Isolation Infrared Spectroscopy and Quantum Chemical Studies on 3-Methyl-1,2-cyclohexanedione*  
Journal of Physical Chemistry A, (114): 1650-1656 2010.

Sankaranarayanan, J.; Rajam, S.; Hadad, C. M.; Gudmundsdottir, A. D.

*The ability of triplet nitrenes to abstract hydrogen atoms*  
Journal of Physical Organic Chemistry, (23): 370-375 2010.

Sarma, B. K.; Manna, D.; Minoura, M.; Mugesh, G.

*Synthesis, Structure, Spirocyclization Mechanism, and Glutathione Peroxidase-like Antioxidant Activity of Stable Spirodiazaselenurane and Spirodiazatellurane*  
Journal of the American Chemical Society, (132): 5364-5374 2010.

Sasanuma, Y.; Ogawa, Y.; Matsumoto, M.

*Predictive elucidation of conformational characteristics and configurational properties of poly(1-methylphosphirane) and poly(1-phenylphosphirane) as a molecular design*  
Physical Chemistry Chemical Physics, (12): 14619-14628 2010.

Sasanuma, Y.; Suzuki, N.

*Structure-Property Relationships of Aromatic Polyesters*  
Kobunshi Ronbunshu, (67): 1-9 2010.

Schiccheri, N.; Pasquini, M.; Piani, G.; Pietraperzia, G.; Becucci, M.; Biczysko, M.; Bloino, J.; Barone, V.  
*Integrated experimental and computational spectroscopy study on pi-stacking interaction: the anisole dimer*  
Physical Chemistry Chemical Physics, (12): 13547-13554 2010.

Schmeisser, M.; Zahl, A.; Scheurer, A.; Puchta, R.; van Eldik, R.

*Ligand Exchange Processes on Solvated Lithium Cations. VI. Determination of Coordination Numbers by Ligand Substitution and Li-7 NMR*  
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (65): 405-413 2010.

Scholz, R.; Hellmann, G.; Rohs, S.; Raabe, G.; Rumsink, J.; Oezdemir, D.; Luche, O.; Hess, T.; Giesen, A. W.; Atodiresei, J.; Lindner, H. J.; Gais, H.-J.

*Experimental and Theoretical Investigation of the Enantiomerization of Lithium alpha-tert-Butylsulfonyl Carbanion Salts and the Determination of Their Structures in Solution and in the Crystal*  
European Journal of Organic Chemistry: 4559-4587 2010.

Schulz, A.; Thomas, J.; Villinger, A.

*Preparation and characterization of [CF<sub>3</sub>SO<sub>3</sub>(SiMe<sub>3</sub>)<sub>2</sub>](+)[B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>](-)*  
Chemical Communications, (46): 3696-3698 2010.

Schulz, A.; Villinger, A.

*Pseudohalonium Ions: [Me<sub>3</sub>Si-X-SiMe<sub>3</sub>](+) (X = CN, OCN, SCN, and NNN)*  
Chemistry-a European Journal, (16): 7276-7281 2010.

Schulz, J.; Gyepes, R.; Cisarova, I.; Stepnicka, P.  
*Synthesis, structural characterisation and bonding in an anionic hexavanadate bearing redox-active ferrocenyl groups at the periphery*  
New Journal of Chemistry, (34): 2749-2756 2010.

Schwoebel, J. A. H.; Wondrousch, D.; Koleva, Y. K.; Madden, J. C.; Cronin, M. T. D.; Schueuermann, G.  
*Prediction of Michael-Type Acceptor Reactivity toward Glutathione*  
Chemical Research in Toxicology, (23): 1576-1585 2010.

Sebastian, S.; Sundaraganesan, N.  
*The spectroscopic (FT-IR, FT-IR gas phase, FT-Raman and UV) and NBO analysis of 4-Hydroxypiperidine by density functional method*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (75): 941-952 2010.

Sedlak, R.; Fanfrlik, J.; Hnyk, D.; Hobza, P.; Lepsik, M.  
*Interactions of Boranes and Carboranes with Aromatic Systems: CCSD(T) Complete Basis Set Calculations and DFT-SAPT Analysis of Energy Components*  
Journal of Physical Chemistry A, (114): 11304-11311 2010.

Selvakumar, K.; Singh, H. B.; Butcher, R. J.  
*Aromatic Ring Strain in Arylselenenyl Bromides: Role in Facile Synthesis of Selenenate Esters via Intramolecular Cyclization*  
Chemistry-a European Journal, (16): 10576-10591 2010.

Semenov, S. G.; Solov'eva, A. G.  
*Cubyl Cations: A Quantum-Chemical Study*  
Russian Journal of General Chemistry, (80): 2314-2316 2010.

Sen, A.; Singh, A.; Ganguly, B.  
*Probing the influence of solvent effects on the conformational behavior of 1,4-diazacyclohexane systems*  
Journal of Molecular Structure, (984): 294-299 2010.

Sen Gupta, S. K.; Prasad, R.  
*Origin and Nature of Transmission Modes of Anomalous Effects of meta-Substituents on the C-13 Chemical Shift of the Carboxyl Carbon ( $\delta(CO)$ ) of Benzoic Acid*  
Australian Journal of Chemistry, (63): 321-328 2010.

Sen, K.; Hackett, J. C.  
*Peroxo-Iron Mediated Deformylation in Sterol 14 alpha-Demethylase Catalysis*  
Journal of the American Chemical Society, (132): 10293-10305 2010.

Seok, W. K.; Klapoetke, T. M.  
*Inorganic and Transition Metal Azides*  
Bulletin of the Korean Chemical Society, (31): 781-788 2010.

Sergeeva, A. P.; Boldyrev, A. I.

*THE CHEMICAL BONDING OF Re<sub>3</sub>Cl<sub>9</sub> AND Re<sub>3</sub>Cl<sub>9</sub>2- REVEALED BY THE ADAPTIVE NATURAL DENSITY PARTITIONING ANALYSES*  
Comments on Inorganic Chemistry, (31): 2-12 2010.

Serpell, C. J.; Kilah, N. L.; Costa, P. J.; Felix, V.; Beer, P. D.  
*Halogen Bond Anion Templated Assembly of an Imidazolium Pseudorotaxane*  
Angewandte Chemie-International Edition, (49): 5322-5326 2010.

Shaik, S.; Wang, Y.; Chen, H.; Song, J.; Meir, R.  
*Valence bond modelling and density functional theory calculations of reactivity and mechanism of cytochrome P450 enzymes: thioether sulfoxidation*  
Faraday Discussions, (145): 49-70 2010.

Shainyan, B. A.; Chipanina, N. N.; Aksamentova, T. N.; Oznobikhina, L. P.; Rosentsveig, G. N.; Rosentsveig, I. B.  
*Intramolecular hydrogen bonds in the sulfonamide derivatives of oxamide, dithioxoamide, and biuret. FT-IR and DFT study, AIM and NBO analysis*  
Tetrahedron, (66): 8551-8556 2010.

Shankar, R.; Kolandaivel, P.; Senthilkumar, K.  
*Reaction Mechanism of Cysteine Proteases Model Compound HSH With Diketone Inhibitor PhCOCOCH<sub>3</sub>-nX<sub>n</sub>, (X = F, Cl, n=0, 1, 2)*  
International Journal of Quantum Chemistry, (110): 1660-1674 2010.

Shao, J.; Shi, R.; Wang, C.; Zhu, X.; Lu, X.  
*Exploration of structure, potential energy surface, and stability of planar C<sub>3</sub>B<sub>3</sub>*  
Journal of Molecular Modeling, (16): 939-950 2010.

Shi, J.; Huang, X.-Y.; Wang, J.-P.; Li, R.  
*A Theoretical Study on C-COOH Homolytic Bond Dissociation Enthalpies*  
Journal of Physical Chemistry A, (114): 6263-6272 2010.

Shieh, M.; Chu, Y.-Y.; Miu, C.-Y.; Wu, P.-F.; Zeng, T.-M.  
*Bimetallic Ru-Cu tellurido complexes: controlled synthesis and electrochemical studies of copper halide-T<sub>e</sub>Ru<sub>5</sub> and Te<sub>2</sub>Ru<sub>4</sub> clusters*  
Dalton Transactions, (39): 1492-1503 2010.

Shieh, M.; Lin, C.-N.; Miu, C.-Y.; Hsu, M.-H.; Pan, Y.-W.; Ho, L.-F.  
*Chromium-Manganese Selenide Carbonyl Complexes: Paramagnetic Clusters and Relevance to C=O Activation of Acetone*  
Inorganic Chemistry, (49): 8056-8066 2010.

Shima, T.; Namura, K.; Kameo, H.; Kakuta, S.; Suzuki, H.  
*Synthesis and Structure of a Novel Ruthenium Hydrido Bis(dihydrogen) Complex with 1,4,7-Trimethyl-1,4,7-triazacyclononane Ligand: A Useful Precursor for Synthesis of Heterometallic Complexes*  
Organometallics, (29): 337-346 2010.

- Shirhatti, P. R.; Wategaonkar, S.  
*Blue shifted hydrogen bond in 3-methylindole center dot CHX<sub>3</sub> complexes (X = Cl, F)*  
Physical Chemistry Chemical Physics, (12): 6650-6659 2010.
- Shiroodi, A.; Zahedi, E.  
*Theoretical study of HF elimination kinetics of ethane fluorides and derivatives [C<sub>2</sub>H<sub>6</sub>-nFn (n=1-4)]*  
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (49): 1579-1585 2010.
- Shishkin, O. V.; Omelchenko, I. V.; Kalyuzhny, A. L.; Paponov, B. V.  
*Intramolecular S center dot center dot center dot O chalcogen bond in thioindirubin*  
Structural Chemistry, (21): 1005-1011 2010.
- Shishkov, I. F.; Sipachev, V. A.; Dem'yanov, P. I.; Dorofeeva, O. V.; Vogt, N.; Vishnevskiy, Y. V.; Vilkov, L. V.  
*An alternative gas-phase electron diffraction and quantum chemical study of nitroethane*  
Journal of Molecular Structure, (978): 41-47 2010.
- Shlykov, S. A.; Giricheva, N. I.; Titov, A. V.; Szwak, M.; Lentz, D.; Girichev, G. V.  
*The structures of tellurium(IV) halides in the gas phase and as solvated molecules*  
Dalton Transactions, (39): 3245-3255 2010.
- Shoji, Y.; Matsuo, T.; Hashizume, D.; Fueno, H.; Tanaka, K.; Tamao, K.  
*A Stable Doubly Hydrogen-Bridged Butterfly-Shaped Diborane(4) Compound*  
Journal of the American Chemical Society, (132): 8258-+ 2010.
- Shubina, T. E.; Clark, T.  
*Catalysis of the Quadricyclane to Norbornadiene Rearrangement by SnCl<sub>2</sub> and CuSO<sub>4</sub>*  
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (65): 347-356 2010.
- Silva, V. H. C.; Camargo, L. T. F. M.; Napolitano, H. B.; Perez, C. N.; Camargo, A. J.  
*Theoretical investigation of the interaction of glycerol with aluminum and magnesium phthalocyanines*  
Journal of Molecular Graphics and Modelling, (29): 206-213 2010.
- Simkowa, I.; Latos-Grazynski, L.; Stepien, M.  
*pi Conjugation Transmitted across a d-Electron Metallocene in Ferrocenothiaporphyrin Macrocycles*  
Angewandte Chemie-International Edition, (49): 7665-7669 2010.
- Simon, P.; de Proft, F.; Jambor, R.; Ruzicka, A.; Dostal, L.  
*Monomeric Organoantimony(I) and Organobismuth(I) Compounds Stabilized by an NCN Chelating Ligand: Syntheses and Structures*  
Angewandte Chemie-International Edition, (49): 5468-5471 2010.
- Singh, N.; Bhattacharya, S.; Noeth, H.  
*Synthesis and characterization of a diorganotin bis(thioacetate)*  
Journal of Molecular Structure, (969): 229-232 2010.

- Singh, N.; Kumar, A.; Prasad, R.; Molloy, K. C.; Mahon, M. F.  
*Syntheses, crystal, photoluminescence and electrochemical investigation of some new phenylmercury(II) dithiocarbamate complexes involving ferrocene*  
Dalton Transactions, (39): 2667-2675 2010.
- Singh, V.; Chauhan, R.; Kumar, A.; Bahadur, L.; Singh, N.  
*Efficient phenylmercury(II) methylferrocenyldithiocarbamate functionalized dye-sensitized solar cells*  
Dalton Transactions, (39): 9779-9788 2010.
- Sircoglou, M.; Bontemps, S.; Mercy, M.; Miqueu, K.; Ladeira, S.; Saffon, N.; Maron, L.; Bouhadir, G.; Bourissou, D.  
*Copper(I) Complexes derived from Mono- and Diphosphino-Boranes: Cu -> B Interactions Supported by Arene Coordination*  
Inorganic Chemistry, (49): 3983-3990 2010.
- Skarmoutsos, I.; Hunt, P. A.  
*Structural and Dynamic Properties of the New Alternative Refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf) in the Liquid State*  
Journal of Physical Chemistry B, (114): 17120-17127 2010.
- Sokolov, A. Y.; Schaefer, H. F., III  
*Coordination Properties of Bridging Diazene Ligands in Unusual Diiron Complexes*  
Organometallics, (29): 3271-3280 2010.
- Sokolov, A. Y.; Sizova, O. V.  
*Quantum-Chemical Study of trans Influence in Gold(I) Linear Complexes*  
Russian Journal of General Chemistry, (80): 1223-1231 2010.
- Solimannejad, M.; Shahbazi, F.; Alkorta, I.  
*A Computational Study of the Potential Energy Surface of Peroxyformic Acid Dimers*  
Journal of Physical Chemistry A, (114): 9388-9393 2010.
- Soloducho, J.; Cabaj, J.; Idzik, K.; Nowakowska-Oleksy, A.; Swist, A.; Lapkowski, M.  
*Synthesis, Structure and Properties of Crowded Symmetric Arylenes*  
Current Organic Chemistry, (14): 1234-1244 2010.
- Song, J.; Zhao, P. S.; Zhang, W. G.  
*Synthesis, Crystal Structure, Spectra Characterization and DFT Studies on a Di-Cycle Pyrazoline Derivative*  
Bulletin of the Korean Chemical Society, (31): 1875-1880 2010.
- Song, P.; Guan, W.; Yan, L.; Liu, C.; Su, Z.  
*Theoretical study on the tetrานuclear endohedral vanadyl carboxylates with guest-switchable redox properties and large polarizability*  
Dalton Transactions, (39): 3706-3713 2010.

- Soralova, S.; Breza, M.  
*DFT study of bis(picolinato-*N,O*)-copper(II) complex*  
Polyhedron, (29): 2440-2444 2010.
- Soras, G.; Psaroudakis, N.; Mousdis, G. A.; Manos, M. J.; Tasiopoulos, A. J.; Aloukos, P.; Couris, S.; Labeguerie, P.; Lipinski, J.; Avramopoulos, A.; Papadopoulos, M. G.  
*Synthesis and non-linear optical properties of some novel nickel derivatives*  
Chemical Physics, (372): 33-45 2010.
- Sordo, T. L.; Menendez, M. I.  
*Subporphyrinoid Systems: A Theoretical Study of the Effects of the Diheteroatom Substitution in Pyrrole Subunits and of the Nature of the Bridging Meso Linkages*  
Journal of Organic Chemistry, (75): 5904-5910 2010.
- Soto-Delgado, J.; Aizman, A.; Domingo, L. R.; Contreras, R.  
*Invariance of electrophilicity of independent fragments. Application to intramolecular Diels-Alder reactions*  
Chemical Physics Letters, (499): 272-277 2010.
- Soto-Delgado, J.; Domingo, L. R.; Contreras, R.  
*Quantitative characterization of group electrophilicity and nucleophilicity for intramolecular Diels-Alder reactions*  
Organic & Biomolecular Chemistry, (8): 3678-3683 2010.
- Sproules, S.; Kapre, R. R.; Roy, N.; Weyhermueller, T.; Wieghardt, K.  
*The molecular and electronic structures of monomeric cobalt complexes containing redox noninnocent o-aminobenzenethiolate ligands*  
Inorganica Chimica Acta, (363): 2702-2714 2010.
- Srivastava, K.; Chakraborty, T.; Singh, H. B.; Singh, U. P.; Butcher, R. J.  
*Isolation and reactivity of an unusually stable organoselenenyl azide*  
Dalton Transactions, (39): 10137-10141 2010.
- Stankovic, S.; Markovic, S.; Gutman, I.; Sretenovic, S.  
*Hydrogen-mediated Stone-Wales isomerization of dicyclopenta[de,mn]anthracene*  
Journal of Molecular Modeling, (16): 1519-1527 2010.
- Starosta, R.; Bazanow, B.; Barszczewski, W.  
*Chalcogenides of the aminomethylphosphines derived from 1-methylpiperazine, 1-ethylpiperazine and morpholine: NMR, DFT and structural studies for determination of electronic and steric properties of the phosphines*  
Dalton Transactions, (39): 7547-7555 2010.
- Steenken, S.; Reynisson, J.  
*DFT calculations on the deprotonation site of the one-electron oxidised guanine-cytosine base pair*  
Physical Chemistry Chemical Physics, (12): 9089-9094 2010.

Stephen, A. D.; Pawar, R. B.; Kumaradhas, P.

*Exploring the bond topological properties and the charge depletion-impact sensitivity relationship of high energetic TNT molecule via theoretical charge density analysis*  
Journal of Molecular Structure-Theochem, (959): 55-61 2010.

Steudel, R.; Steudel, Y.

*Derivatives of cysteine related to the thiosulfate metabolism of sulfur bacteria by the multi-enzyme complex "Sox"-studied by B3LYP-PCM and G3X(MP2) calculations*  
Physical Chemistry Chemical Physics, (12): 630-644 2010.

Steudel, R.; Steudel, Y.

*Reversal of the Relative Stability of the Isomeric Radicals HSO and HOS upon Hydration and Their Reactions with Ozone*  
Journal of Physical Chemistry A, (114): 4437-4445 2010.

Steudel, Y.; Steudel, R.

*Structural Isomerism and Thermodynamic Properties of the Methylzinc Alkoxide Molecules (MeZnOR)(n) (R = Me, 'Bu) and Cations [(MeZnOMe)(n)](+) (n=3, 4) Studied by B3LYP and PCM Calculations*  
Journal of Physical Chemistry A, (114): 6370-6376 2010.

Su, Z.; Qin, S.; Hu, C.; Feng, X.

*Theoretical Investigations on the Mechanism of Hetero-Diels-Alder Reactions of Brassard's Diene and 1, 3-Butadiene Catalyzed by a Tridentate Schiff Base Titanium(IV) Complex*  
Chemistry-a European Journal, (16): 4359-4367 2010.

Subashchandrabose, S.; Krishnan, A. R.; Saleem, H.; Parameswari, R.; Sundaraganesan, N.; Thanikachalam, V.; Manikandan, G.

*Vibrational spectroscopic study and NBO analysis on bis(4-amino-5-mercapto-1,2,4-triazol-3-yl)methane using DFT method*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (77): 877-884 2010.

Subashchandrabose, S.; Krishnan, A. R.; Saleem, H.; Thanikachalam, V.; Manikandan, G.; Erdogan, Y.

*FT-IR, FT-Raman, NMR spectral analysis and theoretical NBO, HOMO-LUMO analysis of bis(4-amino-5-mercapto-1,2,4-triazol-3-yl)ethane by ab initio HF and DFT methods*  
Journal of Molecular Structure, (981): 59-70 2010.

Subramanian, M. K.; Anbarasan, P. M.; Manimegalai, S.

*Molecular structure, vibrational spectroscopic studies and natural bond orbital analysis of 7-amino-4-trifluoromethyl coumarin*  
Pramana-Journal of Physics, (74): 845-850 2010.

Sun, H.; Gong, H.; Liu, H.; Wang, F.; Pan, X.; Su, Z.; Sun, C.; Wang, R.; Huang, X.

*Theoretical study on the structures, isomerization and stability of SiC4 isomers*  
Theoretical Chemistry Accounts, (126): 15-25 2010.

Sun, X.; Du, J.; Zhang, P.; Jiang, G.

*A Systemic DFT Study on Several 5d-Electron Element Dimers: Hf-2, Ta-2, Re-2, W-2, and Hg-2*

Journal of Cluster Science, (21): 619-636 2010.

Sun, Z.; Wang, H.; Xie, Y.; King, R. B.; Schaefer, H. F., III  
*Unsaturation and variable hapticity in binuclear azulene manganese carbonyl complexes*  
Dalton Transactions, (39): 10702-10711 2010.

Suvitha, A.; Venkataraman, N. S.; Mizuseki, H.; Kawazoe, Y.; Ohuchi, N.  
*Theoretical insights into the formation, structure, and electronic properties of anticancer oxaliplatin drug and cucurbit n urils n=5 to 8*  
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (66): 213-218 2010.

Szatylowicz, H.; Krygowski, T. M.  
*Effect of the Substituent and Hydrogen Bond on the Geometry and Electronic Properties of OH and O- Groups in para-Substituted Phenol and Phenolate Derivatives*  
Journal of Physical Chemistry A, (114): 10885-10890 2010.

Szatylowicz, H.; Sadlej-Sosnowska, N.  
*Characterizing the Strength of Individual Hydrogen Bonds in DNA Base Pairs*  
Journal of Chemical Information and Modeling, (50): 2151-2161 2010.

Tafipolsky, M.; Amirjalayer, S.; Schmid, R.  
*Atomistic theoretical models for nanoporous hybrid materials*  
Microporous and Mesoporous Materials, (129): 304-318 2010.

Tai, T. B.; Nguyen, M. T.; Dixon, D. A.  
*Thermochemical Properties and Electronic Structure of Boron Oxides B<sub>n</sub>O<sub>m</sub> (n=5-10, m=1-2) and Their Anions*  
Journal of Physical Chemistry A, (114): 2893-2912 2010.

Takagi, N.; Krapp, A.; Frenking, G.  
*On the nature of homo- and hetero-dinuclear metal-metal quadruple bonds - Analysis of the bonding situation and benchmarking DFT against wave function methods*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 1079-1093 2010.

Takase, M. K.; Fang, M.; Ziller, J. W.; Furche, F.; Evans, W. J.  
*Reduction chemistry of the mixed ligand metallocene [(C<sub>5</sub>Me<sub>5</sub>)(C<sub>8</sub>H<sub>8</sub>)U](2)(μ-C<sub>8</sub>H<sub>8</sub>) with bipyridines*  
Inorganica Chimica Acta, (364): 167-171 2010.

Tan, X.; Li, P.; Wang, W.; Yang, X.; Zheng, G.  
*Quantum Chemical Study on the Mechanism of the Addition Reaction between Germylene and Epoxyethane*  
Journal of the Chilean Chemical Society, (55): 78-80 2010.

Tanak, H.  
*Quantum chemical computational studies on 2-methyl-6-[2-(trifluoromethyl)phenyliminomethyl]phenol*  
Journal of Molecular Structure-Theochem, (950): 5-12 2010.

- Tanak, H.; Yavuz, M.  
*Density functional computational studies on (E)-2-[(2-Hydroxy-5-nitrophenyl)-iminiomethyl]-4-nitrophenolate*  
Journal of Molecular Modeling, (16): 235-241 2010.
- Tang, S.-W.; Feng, J.-D.; Qiu, Y.-Q.; Sun, H.; Wang, F.-D.; Chang, Y.-F.; Wang, R.-S.  
*Electronic Structures and Nonlinear Optical Properties of Highly Deformed Halofullerenes C-3v C<sub>60</sub>F<sub>18</sub> and D-3d C<sub>60</sub>Cl<sub>30</sub>*  
Journal of Computational Chemistry, (31): 2650-2657 2010.
- Tang, S.-W.; Feng, J.-D.; Sun, L.-L.; Wang, F.-D.; Sun, H.; Chang, Y.-F.; Wang, R.-S.  
*Structural stability and electronic property of C<sub>68</sub>X<sub>4</sub> (X = H, F, and Cl) fullerene compounds*  
Journal of Molecular Graphics and Modelling, (28): 891-898 2010.
- Tao, G.-H.; Guo, Y.; Parrish, D. A.; Shreeve, J. n. M.  
*Energetic 1,5-diamino-4H-tetrazolium nitro-substituted azolates*  
Journal of Materials Chemistry, (20): 2999-3005 2010.
- Tao, J.; Li, S.  
*Theoretical study on the mechanism of H-2 activation mediated by two transition metal thiolate complexes: Homolytic for Ir, heterolytic for Rh*  
Dalton Transactions, (39): 857-863 2010.
- Tassell, M. J.; Kaltsoyannis, N.  
*Covalency in AnCp(4) (An = Th-Cm): a comparison of molecular orbital, natural population and atoms-in-molecules analyses*  
Dalton Transactions, (39): 6719-6725 2010.
- Teague, C. M.; Dai, S.; Jiang, D.-e.  
*Computational Investigation of Reactive to Nonreactive Capture of Carbon Dioxide by Oxygen-Containing Lewis Bases*  
Journal of Physical Chemistry A, (114): 11761-11767 2010.
- Tiana, D.; Francisco, E.; Blanco, M. A.; Macchi, P.; Sironi, A.; Martin Pendas, A.  
*Bonding in Classical and Nonclassical Transition Metal Carbonyls: The Interacting Quantum Atoms Perspective*  
Journal of Chemical Theory and Computation, (6): 1064-1074 2010.
- Tobisch, S.  
*Mechanistic Exploration of Intramolecular Aminodiene Hydroamination/Cyclisation Mediated by Constrained Geometry Organoactinide Complexes: A DFT Study*  
Chemistry-a European Journal, (16): 3441-3458 2010.
- Tobisch, S.  
*Mechanistic Investigation of Organolanthanide-Mediated Hydroamination of Conjugated Aminodienes: A Comprehensive Computational Assessment of Various Routes for Diene Activation*

Chemistry-a European Journal, (16): 13814-13823 2010.

Toledo, L.; Masgrau, L.; Marechal, J.-D.; Lluch, J. M.; Gonzalez-Lafont, A.

*Insights into the Mechanism of Binding of Arachidonic Acid to Mammalian 15-Lipoxygenases*  
Journal of Physical Chemistry B, (114): 7037-7046 2010.

Tong, J.; Li, Y.; Wu, D.; Cui, S.-H.; Li, Z.-R.; Huang, X.-R.

*Dipole-bound states of the alkali-superhalogen anions: LiBeX<sub>3</sub>- (X = F, Cl, Br)*  
Chemical Physics Letters, (496): 20-24 2010.

Tong, J.; Li, Y.; Wu, D.; Li, Z.-R.; Huang, X.-R.

*Lithium Bonding Interaction Hyperpolarizabilities of Various Li-Bond Dimers*  
Journal of Physical Chemistry A, (114): 5888-5893 2010.

Tong, S.; Ma, C.; Ge, M.; Wang, W.; Wang, D.

*Experimental and theoretical study for substituent effects of three 2-bromothiophene derivatives*  
Journal of Molecular Structure, (978): 108-113 2010.

Tonner, R.; Lein, M.; Wesendrup, R.; Schwerdtfeger, P.

*A systematic density functional and wavefunction-based study on dicarboxyl dianions -O2C-R-CO2 (-) with R = C-2, C2X2, C2X4, and C6X4 (X = H, F)*  
Theoretical Chemistry Accounts, (126): 129-138 2010.

Tormena, C. F.; Lacerda, V.; de Oliveira, K. T.

*Revisiting the Stability of endo/exo Diels-Alder Adducts between Cyclopentadiene and 1,4-benzoquinone*  
Journal of the Brazilian Chemical Society, (21): 112-118 2010.

Torrent-Sucarrat, M.; De Proft, F.; Ayers, P. W.; Geerlings, P.

*On the applicability of local softness and hardness*  
Physical Chemistry Chemical Physics, (12): 1072-1080 2010.

Tosta, M. M.; Mora, J. R.; Cordova, T.; Chuchani, G.

*Joint Experimental and DFT Study of the Gas-Phase Unimolecular Elimination Kinetic of Methyl Trifluoropyruvate*  
Journal of Physical Chemistry A, (114): 7892-7897 2010.

Tosta, M. M.; Mora, J. R.; Cordova, T.; Chuchani, G.

*Quantum chemical calculations of the homogeneous, unimolecular, gas-phase elimination kinetics of primary alkyl acetates and (dimethylamino)alkyl acetates: Neighboring group participation in 4-(dimethylamino)-1-butyl acetate*  
Journal of Molecular Structure-Theochem, (952): 46-55 2010.

Trabolsi, A.; Khashab, N.; Fahrenbach, A. C.; Friedman, D. C.; Colvin, M. T.; Coti, K. K.; Benitez, D.; Tkatchouk, E.; Olsen, J.-C.; Belowich, M. E.; Carmielli, R.; Khatib, H. A.; Goddard, W. A., III; Wasielewski, M. R.; Stoddart, J. F.

*Radically enhanced molecular recognition*  
Nature Chemistry, (2): 42-49 2010.

Trindade, A. F.; Andre, V.; Teresa Duarte, M.; Veiros, L. F.; Gois, P. M. P.; Afonso, C. A. M.

*Selective arylation of aldehydes with di-rhodium(II)/NHC catalysts*

Tetrahedron, (66): 8494-8502 2010.

Truong Ba, T.; Minh Tho, N.

*Thermochemical properties, electronic structure and bonding of mixed lithium boron clusters*

*(B<sub>n</sub>Li, n=1-8) and their anions*

Chemical Physics, (375): 35-45 2010.

Truong Ba, T.; Pham Vu, N.; Minh Tho, N.

*Structure and stability of aluminium doped lithium clusters (Li<sub>n</sub>Al<sub>0/+</sub>, n=1-8): a case of the phenomenological shell model*

Physical Chemistry Chemical Physics, (12): 11477-11486 2010.

Trzewik, B.; Seidler, T.; Broclawik, E.; Stadnicka, K.

*Mechanisms of reactions conducted on alpha-amido-alpha-aminonitrones, determined based on the structures of their crystalline products and DFT calculations*

New Journal of Chemistry, (34): 2220-2228 2010.

Tsipis, A. C.

*Unveiling the Nature of Binding Interactions of Acetylene and Ethylene with Triangular Coinage Metal Clusters: A DFT Computational Study*

Organometallics, (29): 354-363 2010.

Tsivion, E.; Gerber, R. B.

*Predicted compounds of radon with acetylene and water*

Physical Chemistry Chemical Physics, (12): 11791-11794 2010.

Turecek, F.; Chung, T. W.; Moss, C. L.; Wyer, J. A.; Ehlerding, A.; Holm, A. I. S.; Zettergren, H.; Nielsen, S. B.; Hvelplund, P.; Chamot-Rooke, J.; Bythell, B.; Paizs, B.

*The Histidine Effect. Electron Transfer and Capture Cause Different Dissociations and Rearrangements of Histidine Peptide Cation-Radicals*

Journal of the American Chemical Society, (132): 10728-10740 2010.

Uhl, W.; Rohling, M.; Wuerthwein, E.-U.; Ghavtadze, N.; Bergander, K.

*Facile Synthesis of an Unsaturated Spiro Germane by Hydroalumination and Intramolecular 1,1-Carbalumination*

Organometallics, (29): 5236-5240 2010.

Urankar, D.; Pinter, B.; Pevec, A.; De Proft, F.; Turel, I.; Kosmrlj, J.

*Click-Triazole N2 Coordination to Transition-Metal Ions Is Assisted by a Pendant Pyridine Substituent*

Inorganic Chemistry, (49): 4820-4829 2010.

Uribe, E. A.; Daza, M. C.; Villaveces, J. L.; Delgado, S. A.

*On the Nature of Copper-Hydrogen Bonding: AIM and NBO Analysis of CuH<sub>n</sub> (1 <= n <= 6) Complexes*

International Journal of Quantum Chemistry, (110): 524-531 2010.

Vallejos, M. A.; Angelina, E. L.; Peruchena, N. M.

*Bifunctional Hydrogen Bonds in Monohydrated Cycloether Complexes*

Journal of Physical Chemistry A, (114): 2855-2863 2010.

Vallet, V.; Fischer, A.; Szabo, Z.; Grenthe, I.

*The structure and bonding of Y, Eu, U, Am and Cm complexes as studied by quantum chemical methods and X-ray crystallography*

Dalton Transactions, (39): 7666-7672 2010.

Van Damme, S.; Bultinck, P.

*3D QSAR based on conceptual DFT molecular fields: Antitubercular activity*

Journal of Molecular Structure-Theochem, (943): 83-89 2010.

Van Doren, J. M.; Condon, L. R.; DeSouza-Goding, A.; Miller, T. M.; Bopp, J. C.; Viggiano, A. A.

*Electron Affinity of trans-2-C4F8 from Electron Attachment-Detachment Kinetics*

Journal of Physical Chemistry A, (114): 1420-1426 2010.

van Severen, M.-C.; Gourlaouen, C.; Parisel, O.

*Application of the Topological Analysis of the Electronic Localization Function to Archetypical [Pb(II)L-n](p) Complexes: The Bonding of Pb<sup>2+</sup> Revisited*

Journal of Computational Chemistry, (31): 185-194 2010.

Varadwaj, P. R.

*Hydrogen bonding interactions in PN center dot center dot center dot HX complexes: DFT and ab initio studies of structure, properties and topology*

Journal of Molecular Modeling, (16): 965-974 2010.

Varga, Z.; Groen, C. P.; Kolonits, M.; Hargittai, M.

*Curious matrix effects: a computational, electron diffraction, and vibrational spectroscopic study of dysprosium triiodide*

Dalton Transactions, (39): 6221-6230 2010.

Varga, Z.; Kolonits, M.; Hargittai, M.

*Gas-Phase Structures of Iron Trihalides: A Computational Study of all Iron Trihalides and an Electron Diffraction Study of Iron Trichloride*

Inorganic Chemistry, (49): 1039-1045 2010.

Varga, Z.; Vest, B.; Schwerdtfeger, P.; Hargittai, M.

*Molecular Geometry of Vanadium Dichloride and Vanadium Trichloride: A Gas-Phase Electron Diffraction and Computational Study*

Inorganic Chemistry, (49): 2816-2821 2010.

Vaz, P. D.; Nolasco, M. M.; Gil, F. P. S. C.; Ribeiro-Claro, P. J. A.; Tomikinson, J.

*Hydrogen-Bond Dynamics of C-H center dot center dot center dot O Interactions: The Chloroform center dot center dot center dot Acetone Case*

Chemistry-a European Journal, (16): 9010-9017 2010.

Vece, V.; Ricci, J.; Poulain-Martini, S.; Nava, P.; Carissan, Y.; Humbel, S.; Dunach, E.  
*In-III-Catalysed Tandem C-C and C-O Bond Formation between Phenols and Allylic Acetates*  
European Journal of Organic Chemistry: 6239-6248 2010.

Veiro, L. F.; Honzicek, J.; Romao, C. C.; Calhorda, M. J.  
*The role of cyclopentadienyl versus indenyl in Mo(II) spirodiene complexes reactivity: A DFT mechanistic study*  
Inorganica Chimica Acta, (363): 555-561 2010.

Victoria Roux, M.; Notario, R.; Foces-Foces, C.; Temprado, M.; Ros, F.; Emel'yanenko, V. N.; Verevkin, S. P.  
*Experimental and Computational Thermochemical Study and Solid-Phase Structure of 5,5-Dimethylbarbituric Acid*  
Journal of Physical Chemistry A, (114): 3583-3590 2010.

Vila, A.; Mosquera, R. A.  
*On the non-planarity of 1,3-dioxole and 1,3-dioxolane*  
Chemical Physics Letters, (488): 17-21 2010.

Villinger, A.; Schulz, A.  
*Binary Bismuth(III) Azides: Bi(N-3)(3), [Bi(N-3)(4)](-), and [Bi(N-3)(6)](3-)*  
Angewandte Chemie-International Edition, (49): 8017-8020 2010.

Voehringer-Martinez, E.; Toro-Labbe, A.  
*The Role of Water in the Proton Transfer Reaction Mechanism in Tryptophan*  
Journal of Computational Chemistry, (31): 2642-2649 2010.

Wadnerkar, N.; Kalamse, V.; Chaudhari, A.  
*Hydrogen Uptake Capacity of C<sub>2</sub>H<sub>4</sub>Sc and its Ions: A Density Functional Study*  
Journal of Computational Chemistry, (31): 1656-1661 2010.

Wan, L.; Zhang, Y.; Qi, D.; Jiang, J.  
*Structures and properties of 1,8,15,22-tetrasubstituted phthalocyaninato zinc and nickel complexes: Substitution and axially coordination effects study based on density functional theory calculations*  
Journal of Molecular Graphics and Modelling, (28): 842-851 2010.

Wang, C.; Olson, M. A.; Fang, L.; Benitez, D.; Tkatchouk, E.; Basu, S.; Basuray, A. N.; Zhang, D.; Zhu, D.; Goddard, W. A.; Stoddart, J. F.  
*Isolation by crystallization of translational isomers of a bistable donor-acceptor [2]catenane*  
Proceedings of the National Academy of Sciences of the United States of America, (107): 13991-13996 2010.

Wang, F.; Meng, Q.; Li, M.  
*Mechanism of Rhodium-Catalyzed Hydroacylation of Propylene Using Formaldehyde: A Computational Study*  
International Journal of Quantum Chemistry, (110): 850-859 2010.

- Wang, H.-Q.; Kuang, X.-Y.; Li, H.-F.  
*Density functional study of structural and electronic properties of bimetallic copper-gold clusters: comparison with pure and doped gold clusters*  
Physical Chemistry Chemical Physics, (12): 5156-5165 2010.
- Wang, J.-Q.; Wahl, B.; Faessler, T. F.  
*[Ag(Sn-9-Sn-9)](5-): A Homoleptic Silver Complex of A Dimeric Sn-9 Zintl Anion*  
Angewandte Chemie-International Edition, (49): 6592-6595 2010.
- Wang, L.-F.  
*Coordination and morphology of metal/polyetherurethane complexes*  
European Polymer Journal, (46): 2372-2380 2010.
- Wang, L.-M.; Averkiev, B. B.; Ramilowski, J. A.; Huang, W.; Wang, L.-S.; Boldyrev, A. I.  
*Planar to Linear Structural Transition in Small Boron-Carbon Mixed Clusters: CxB5-x- (x=1-5)*  
Journal of the American Chemical Society, (132): 14104-14112 2010.
- Wang, M.; Chen, S.; Xia, Y.; Zhang, Y.; Huang, W.; Zheng, J.; Li, Z.  
*Nanoassemblies of Colloidal Gold Nanoparticles by Oxygen-Induced Inorganic Ligand Replacement*  
Langmuir, (26): 9351-9356 2010.
- Wang, Q.; Gao, J.; Liu, Y.; Liu, C.  
*Validating a new proton shuttle reaction pathway for formation of the peptide bond in ribosomes: A theoretical investigation*  
Chemical Physics Letters, (501): 113-117 2010.
- Wang, S.-G.; Qiu, Y.-X.; Schwarz, W. H. E.  
*Antibond Breaking-The Formation and Decomposition of He@Adamantane: Descriptions, Explanations, and Meaning of Concepts*  
Chemistry-a European Journal, (16): 9107-9116 2010.
- Wang, T.; Bowie, J. H.  
*Radical routes to interstellar glycolaldehyde. The possibility of stereoselectivity in gas-phase polymerization reactions involving CH<sub>2</sub>O and (CH<sub>2</sub>OH)-C-center dot*  
Organic & Biomolecular Chemistry, (8): 4757-4766 2010.
- Wang, W.; Zhang, Y.; Ji, B.  
*The Nature of the Bond-Length Change Upon Molecule Complexation*  
Collection of Czechoslovak Chemical Communications, (75): 243-256 2010.
- Wang, W.; Zhang, Y.; Ji, B.  
*On the Difference of the Properties between the Blue-Shifting Halogen Bond and the Blue-Shifting Hydrogen Bond*  
Journal of Physical Chemistry A, (114): 7257-7260 2010.
- Wang, X.; Sun, G.; Sun, S.; Liu, C.; Qiu, Y.; Fu, Q.

*Structures and properties of metal-free and magnesium tetrathieno[2,3-*b*]porphyrazine investigated using density functional theory*  
Science China-Chemistry, (53): 1746-1753 2010.

Wang, Y.; Liu, C.  
*De localization and electron transfer in polypeptides with different secondary structures*  
Journal of Molecular Structure-Theochem, (948): 78-82 2010.

Wang, Y.; Wu, J. I. C.; Li, Q.; Schleyer, P. v. R.  
*Aromaticity and Relative Stabilities of Azines*  
Organic Letters, (12): 4824-4827 2010.

Wang, Y.-F.; Chen, W.; Yu, G.-T.; Li, Z.-R.; Sun, C.-C.  
*Novel Metal-[Metal Oxide]-Nonmetal Sandwich-Like Superalkali Compounds Li<sub>3</sub>OMC<sub>5</sub>H<sub>5</sub> (M = Be, Mg, and Ca): How to Increase the Aromaticity of Li-3(+) Ring?*  
International Journal of Quantum Chemistry, (110): 1953-1963 2010.

Wang, Y.-F.; Li, Y.; Li, Z.-R.; Ma, F.; Wu, D.; Sun, C.-C.  
*Perfluorinated exohedral potassium-metallocfullerene K center dot center dot center dot CnFn (n = 20 or 60): partial interior and surface excess electron state*  
Theoretical Chemistry Accounts, (127): 641-650 2010.

Wang, Z.; Zheng, B.; Yu, X.; Li, X.; Yi, P.  
*Structure, properties, and nature of the pyridine-XY (X, Y=F, Cl, Br) complexes: An ab initio study*  
Journal of Chemical Physics, (132) 2010.

Weber, J.; Guenne, J. S. A. D.  
*Calculation of NMR parameters in ionic solids by an improved self-consistent embedded cluster method*  
Physical Chemistry Chemical Physics, (12): 583-603 2010.

Wei, X.-G.; Sun, X.-M.; Wu, X.-P.; Ren, Y.; Wong, N.-B.; Li, W.-K.  
*Enhanced Reactivity of RC=CZ(-) (R = H and Cl; Z = O, S, and Se) and the Influence of Leaving Group on the alpha-Effect in the E2 Reactions*  
Journal of Organic Chemistry, (75): 4212-4217 2010.

Welker, M.; Woodward, S.; Veiros, L. F.; Calhorda, M. J.  
*Chemoselectivity as a Delineator of Cuprate Structure in Catalytic 1,4-Addition of Diorganozinc Reagents to Michael Acceptors*  
Chemistry-a European Journal, (16): 5620-5629 2010.

Wendler, K.; Thar, J.; Zahn, S.; Kirchner, B.  
*Estimating the Hydrogen Bond Energy*  
Journal of Physical Chemistry A, (114): 9529-9536 2010.

Werkema, E. L.; Andersen, R. A.; Maron, L.; Eisenstein, O.  
*The reaction of bis(1,2,4-tri-*t*-butylcyclopentadienyl)ceriumbenzyl, Cp'2CeCH<sub>2</sub>Ph, with methylhalides: a metathesis reaction that does not proceed by a metathesis transition state*

Dalton Transactions, (39): 6648-6660 2010.

Woebkenberg, P. H.; Labram, J. G.; Swiecicki, J.-M.; Parkhomenko, K.; Sredojevic, D.; Gisselbrecht, J.-P.; de Leeuw, D. M.; Bradley, D. D. C.; Djukic, J.-P.; Anthopoulos, T. D.

*Ambipolar organic transistors and near-infrared phototransistors based on a solution-processable squarilium dye*

Journal of Materials Chemistry, (20): 3673-3680 2010.

Wohlthat, S.; Reimers, J. R.; Hush, N. S.

*Accurate and computationally efficient third-nearest-neighbor tight-binding model for large graphene fragments*

Physical Review B, (81) 2010.

Wolf, R.; Plois, M.; Hepp, A.

*Neutral and Cationic Hydridoruthenium Tetrakiscarbene Complexes*

European Journal of Inorganic Chemistry: 918-925 2010.

Wolf, R.; Plois, M.; Hepp, A.

*Neutral and Cationic Hydridoruthenium Tetrakiscarbene Complexes*

European Journal of Inorganic Chemistry: 918-925 2010.

Won, Y. S.; Park, S. S.

*DFT Study on the Gas Phase Decomposition of Tungsten Imido Guanidinate Complex W(NiPr)Cl-*

*3[iPrNC(NMe<sub>2</sub>)NiPr] for Chemical Vapor Deposition of Tungsten Carbonitride Films*

Bulletin of the Korean Chemical Society, (31): 2416-2418 2010.

Wu, J.

*Theoretical investigations of the nature of interaction of Br-2 with hydrogen halide*

Journal of Molecular Structure-Theochem, (958): 59-63 2010.

Wu, J.; Sun, Z.; Li, X.; Chen, L.; Tian, M.

*Molecular geometries, electronic properties, and vibrational spectroscopic studies of endohedral metallofullerenes TM@C-24 and TM@C<sub>24</sub>H<sub>12</sub> (TM = Cr, Mo, and W)*

Structural Chemistry, (21): 673-680 2010.

Wu, J.; Yan, H.; Jin, Y.; Dai, G.; Zhong, A.

*Characteristics and nature of the intermolecular interactions between pyridine and various hydrides: A theoretical study*

Journal of Molecular Structure-Theochem, (944): 70-75 2010.

Wu, J. Y.; Yan, H.; Jin, Y. X.; Dai, G. L.; Zhong, A. G.

*Characteristics and nature of the intermolecular interactions between pyridine and various hydrides: A theoretical study*

Journal of Molecular Structure-Theochem, (944): 70-75 2010.

Wu, W.; Shaik, S.; Saunders, W. H., Jr.

*VBSCF Calculations on the Bimolecular (E2) Elimination Reaction. The Nature of the Transition State*

Journal of Organic Chemistry, (75): 3722-3728 2010.

Wu, X.; Qin, Z.; Xie, H.; Cong, R.; Wu, X.; Tang, Z.; Fan, H.

*Photoelectron Imaging and Theoretical Studies of Group 11 Cyanides MCN (M = Cu, Ag, Au)*

Journal of Physical Chemistry A, (114): 12839-12844 2010.

Wu, X.-P.; Wei, X.-G.; Sun, X.-M.; Ren, Y.; Wong, N.-B.; Li, W.-K.

*Theoretical study on the role of cooperative solvent molecules in the neutral hydrolysis of ketene*

Theoretical Chemistry Accounts, (127): 493-506 2010.

Wu, Y.; Jin, L.; Xue, Y.; Lee, I.-M.; Kim, C. K.

*Mechanisms of Norbornadiene Dimerization to Binor-s Using Cationic Co-I, Rh-I, and Ir-I Catalysts*

Journal of Computational Chemistry, (31): 2248-2257 2010.

Wu, Y. B.; Jiang, J. L.; Zhang, R. W.; Wang, Z. X.

*Computationally Designed Families of Flat, Tubular, and Cage Molecules Assembled with "Starbenzene" Building Blocks through Hydrogen-Bridge Bonds*

Chemistry-a European Journal, (16): 1271-1280 2010.

Xie, M.-X.; Xu, X.; Huang, X.-X.

*Theoretical Studies on the Cu-Cu Interaction and Stability of [Cu-a(Ph(2)Ppy)(b)(CH3CN)(c)](a+)*  
*(a=1 similar to 2, b=1 similar to 3, c=0 similar to 2)*

Chinese Journal of Structural Chemistry, (29): 668-675 2010.

Xie, X.; Shen, W.; Fu, Y.; Li, M.

*DFT study of conductive properties of three polymers formed by bicyclic furans*

Molecular Simulation, (36): 836-846 2010.

Xing, D.; Tan, X.; Zhang, C.; Bu, Y.

*Theoretical investigation on the structural and electronic properties of complexes formed by N7,N9-dimethylguaninium and different anions*

Journal of Molecular Structure-Theochem, (939): 82-90 2010.

Xiong, R.; Keffer, D. J.; Fuentes-Cabrera, M.; Nicholson, D. M.; Michalkova, A.; Petrova, T.; Leszczynski, J.; Odbadrakh, K.; Doss, B. L.; Lewis, J. P.

*Effect of Charge Distribution on RDX Adsorption in IRMOF-10*

Langmuir, (26): 5942-5950 2010.

Xiong, R.; Odbadrakh, K.; Michalkova, A.; Luna, J. P.; Petrova, T.; Keffer, D. J.; Nicholson, D. M.; Fuentes-Cabrera, M. A.; Lewis, J. P.; Leszczynski, J.

*Evaluation of functionalized isoreticular metal organic frameworks (IRMOFs) as smart nanoporous preconcentrators of RDX*

Sensors and Actuators B-Chemical, (148): 459-468 2010.

Xu, D.; Hawk, L. L.; Loveless, D. M.; Jeon, S. L.; Craig, S. L.

*Mechanism of Shear Thickening in Reversibly Cross-Linked Supramolecular Polymer Networks*

Macromolecules, (43): 3556-3565 2010.

Xu, J.; Yang, H.-Q.; Qin, S.; Hu, C.-W.  
*THEORETICAL STUDY ON METHANE HYDROXYLATION BY MIMIC METHANE MONOOXYGENASE  
WITH bis(mu-OXO)DIMANGANESE CORE*  
Journal of Theoretical & Computational Chemistry, (9): 233-247 2010.

Xu, L.; Li, Q.-s.; Xie, Y.; King, R. B.; Schaefer, H. F., III  
*Binuclear fluoroborylene manganese carbonyls*  
Inorganica Chimica Acta, (363): 3538-3549 2010.

Xu, L.; Li, Q.-s.; Xie, Y.; King, R. B.; Schaefer, H. F., III  
*Fe-3(BF)(3)(CO)(8) structures with face-semibridging fluoroborylene ligands and a bicapped tetrahedral Fe3B3 cluster isoelectronic with Os-6(CO)(18)*  
New Journal of Chemistry, (34): 2813-2821 2010.

Xu, L.; Lv, J.; Sang, P.; Zou, J.-W.; Yu, Q.-S.  
*DFT model investigations on copper(II) chloride complexes: Halogen bonding of pyridyl bromine of CuCl<sub>2</sub>(NH<sub>3</sub>)(NC<sub>5</sub>H<sub>4</sub>Br-3) with several metal ligands*  
Journal of Molecular Structure-Theochem, (953): 170-174 2010.

Xu, L.; Zou, J.-W.; Yu, Q.-S.; Sang, P.  
*Computational Insights into Halogen Bonding Between P-Cl Contact and Several Electron Donors*  
International Journal of Quantum Chemistry, (110): 1245-1251 2010.

Xu, R.; Klatt, G.; Wadeppohl, H.; Koeppel, H.  
*Hydrogen Scrambling in [(C<sub>5</sub>R<sub>5</sub>)(L)M(H)(C<sub>2</sub>H<sub>4</sub>)](+) (M = Co, Rh). Relation of Experimental Kinetic Data to the Barriers of the Elementary Reaction Steps*  
Inorganic Chemistry, (49): 3289-3296 2010.

Xu, T.; Yang, Q.; Li, D.; Dong, J.; Yu, Z.; Li, Y.  
*Iron(III)-Catalyzed Cyclization of Alkynyl Aldehyde Acetals: Experimental and Computational Studies*  
Chemistry-a European Journal, (16): 9264-9272 2010.

Xu, W. Z.; Ren, F. D.; Ren, J.; Liu, S. N.; Yue, Y.; Wang, W. L.; Chen, S. S.  
*A UB3LYP and UMP2 theoretical investigation on unusual cation-pi interaction between the triplet state HB=BH (3 Sigma(-)(g)) and H+, Li+, Na+, Be2+ or Mg2+*  
Journal of Molecular Modeling, (16): 615-627 2010.

Xu, W.-z.; Ren, F.-d.; Ren, J.; Liu, S.-n.; Yue, Y.; Wang, W.-l.; Chen, S.-s.  
*A UB3LYP and UMP2 theoretical investigation on unusual cation-pi interaction between the triplet state HB=BH (3 Sigma(-)(g)) and H+, Li+, Na+, Be2+ or Mg2+*  
Journal of Molecular Modeling, (16): 615-627 2010.

Xu, Y.; Zhao, F.; Zhang, Y.; Gu, Y.; Liu, T.; Cui, J.  
*Potential High-Energy Pentazolides: HB(N-5)(3)M-1 similar to 2(N-5)(3)BH (M = Be, Mg, Ca, Zn, and Cd)*  
International Journal of Quantum Chemistry, (110): 1235-1244 2010.

Xue, C.; He, G.; Fu, C.; Xue, L.; Lin, Z.; Ma, S.  
*The Reaction of Carboxylic Acid Esters with RfMgBr: A Convenient Synthesis of Perfluoroalkyl Ketones*  
European Journal of Organic Chemistry: 7012-7019 2010.

Xue, Y.; Mansoori, G. A.  
*Self-Assembly of Diamondoid Molecules and Derivatives (MD Simulations and DFT Calculations)*  
International Journal of Molecular Sciences, (11): 288-303 2010.

Xue, Z.-M.; Ding, J.; Zhou, W.; Chen, C.-H.  
*Density functional theory study on LBDOB and its derivatives: Electronic structures, energies, and molecular properties*  
Electrochimica Acta, (55): 3838-3844 2010.

Xue, Z.-M.; Zhou, W.; Ding, J.; Chen, C.-H.  
*Electronic structures and molecular properties of FLBDOB and its derivatives: A combined experimental and theoretical study*  
Electrochimica Acta, (55): 5342-5348 2010.

Yahia, A.; Arnold, P. L.; Love, J. B.; Maron, L.  
*The Effect of the Equatorial Environment on Oxo-Group Silylation of the Uranyl Dication: A Computational Study*  
Chemistry-a European Journal, (16): 4881-4888 2010.

Yahia, A.; Kramer, M. U.; Okuda, J.; Maron, L.  
*C-C coupling reaction of pyridine derivatives at the dimethyl rare-earth metal cation [YMe<sub>2</sub>(THF)(5)](+): A DFT investigation*  
Journal of Organometallic Chemistry, (695): 2789-2793 2010.

Yan, D.; Lu, J.; Ma, J.; Wei, M.; Evans, D. G.; Duan, X.  
*Benzocarbazole anions intercalated layered double hydroxide and its tunable fluorescence*  
Physical Chemistry Chemical Physics, (12): 15085-15092 2010.

Yan, D.; Lu, J.; Ma, J.; Wei, M.; Qin, S.; Chen, L.; Evans, D. G.; Duan, X.  
*Thin film of coumarin-3-carboxylate and surfactant co-intercalated layered double hydroxide with polarized photoluminescence: a joint experimental and molecular dynamics study*  
Journal of Materials Chemistry, (20): 5016-5024 2010.

Yang, J.; Del Rosal, I.; Fasulo, M.; Sangtrirutnugul, P.; Maron, L.; Tilley, T. D.  
*Nickel Complexes with Bis(8-quinolyl)silyl Ligands. An Unusual Ni<sub>3</sub>Si<sub>2</sub> Cluster Containing Six-Coordinate Silicon*  
Organometallics, (29): 5544-5550 2010.

Yang, J.-h.; Ren, F.-d.  
*A (U)MP2(full) and (U)CCSD(T) theoretical investigation on the substituent effect on the cation-pi interactions between Na<sup>+</sup> and LCCL (L = -H, -CH<sub>3</sub>, -OH, -F, -Cl, CO, NN, CN-, NC- and OH-)*  
Journal of Molecular Structure-Theochem, (956): 1-9 2010.

Yang, Q.; Xie, B.; Li, Q.; Zhao, K.  
*Density Functional Theory Study of Hydrogen Bonding Dimers with 4-Pyridinecarboxylic Acid Hydrazine*  
Chinese Journal of Chemistry, (28): 1857-1863 2010.

Yang, Y.  
*Hexacoordinate Bonding and Aromaticity in Silicon Phthalocyanine*  
Journal of Physical Chemistry A, (114): 13257-13267 2010.

Yang, Y.; Liu, Y.  
*Hydrogen Bond of Radicals: Interaction of HNO with HCO, HNO, and HOO*  
International Journal of Quantum Chemistry, (110): 1264-1272 2010.

Yavuz, M.; Tanak, H.  
*Density functional modelling studies on N-2-Methoxyphenyl-2-oxo-5-nitro-1-benzylidenemethylamine*  
Journal of Molecular Structure-Theochem, (961): 9-16 2010.

Yi, Y.; Lee, Y. M.; Park, Y.; Kim, J. W.  
*Gap state formation by interfacial interaction between Al and 8-hydroxyquinolatolithium*  
Physical Chemistry Chemical Physics, (12): 9441-9444 2010.

Yim, W.-L.; Tse, J. S.; Iitaka, T.  
*Pressure-Induced Intermolecular Interactions in Crystalline Silane-Hydrogen*  
Physical Review Letters, (105) 2010.

Yongye, A. B.; Giulianotti, M. A.; Nefzi, A.; Houghten, R. A.; Martinez-Mayorga, K.  
*Conformational landscape of platinum(II)-tetraamine complexes: DFT and NBO studies*  
Journal of Computer-Aided Molecular Design, (24): 225-235 2010.

Yu, F.; Wu, L.-x.; Zhou, X.-g.; Liu, S.-l.  
*Mechanistic Investigation on the Reaction of O- with CH<sub>3</sub>CN Using Density Functional Theory*  
Chinese Journal of Chemical Physics, (23): 643-648 2010.

Yu, S.; Zeng, Q.; Yang, S.; Yang, M.  
*A first-principles study of methylcyclohexane adsorption on Pt-4 clusters*  
Journal of Physics B-Atomic Molecular and Optical Physics, (43) 2010.

Yu, S.-Q.; Jia, X.-F.; Dong, L.-H.; Yin, Y.-S.  
*Structures and Magnetic Properties of Fe<sub>6-x</sub>Al<sub>x</sub> Clusters*  
Acta Physico-Chimica Sinica, (26): 1391-1395 2010.

Yuan, H.; Cao, C.; Gao, S.  
*Topological-quantum Approach and Its Application to the Property Estimation of Compounds Containing Group C=O or N=O*  
Acta Chimica Sinica, (68): 2091-2098 2010.

Yuan, X.-X.; Wang, Y.-F.; Wang, X.; Chen, W.; Fossey, J. S.; Wong, N.-B.

*An ab initio and AIM investigation into the hydration of 2-thioxanthine*  
Chemistry Central Journal, (4) 2010.

Yurkerwich, K.; Coleman, F.; Parkin, G.  
*Bis(2-mercapto-1-R-imidazolyl) hydroborato complexes of aluminium, gallium, indium and thallium: compounds possessing gallium-gallium bonds and a trivalent thallium alkyl*  
Dalton Transactions, (39): 6939-6942 2010.

Yuste, C.; Ferrando-Soria, J.; Cangussu, D.; Fabelo, O.; Ruiz-Perez, C.; Marino, N.; De Munno, G.; Stiriba, S.-E.; Ruiz-Garcia, R.; Cano, J.; Lloret, F.; Julve, M.  
*Topological control of the spin coupling in dinuclear copper(II) complexes with meta- and para-phenylenediamine bridging ligands*  
Inorganica Chimica Acta, (363): 1984-1994 2010.

Zahedi, E.; Ali-Asgari, S.; Keley, V.  
*NBO and NICS analysis of the allylic rearrangements (the Cope and 3-aza-Cope rearrangements) of hexa-1,5-diene and N-vinylprop-2-en-1-amine: A DFT study*  
Central European Journal of Chemistry, (8): 1095-1102 2010.

Zakarianezhad, M.; Habibi-Khorassani, S. M.; Ebrahimi, A.; Maghsoodlou, M. T.; Ghasempour, H.  
*NMR Study, Theoretical Calculations for Assignment of the Z- and E-Isomers, and Kinetics Investigation of Stable Phosphorus Ylides Involving a 2-Mercapto-4,6-dimethyl Pyrimidine Heteroatom Chemistry*, (21): 462-474 2010.

Zanti, G.; Peeters, D.  
*DFT Study of Bimetallic Palladium-Gold Clusters PdnAum of Low Nuclearities (n plus m <= 14)*  
Journal of Physical Chemistry A, (114): 10345-10356 2010.

Zeckert, K.; Zahn, S.; Kirchner, B.  
*Tin-Lanthanoid donor-acceptor bonds*  
Chemical Communications, (46): 2638-2640 2010.

Zeinahnezhad, A.; Nori-Shargh, D.; Abbasi-Bakhtiari, Z.; Boggs, J. E.  
*Ab initio and NBO analysis of the conformational properties of 1,2-oxathiane mono-S-oxide, 1,2-dithiane mono-S-oxide and 1,2-thiaselenane mono-S-oxide*  
Journal of Molecular Structure-Theochem, (947): 52-57 2010.

Zeng, Q.; Wang, X.; Yang, M. L.; Fu, H. B.  
*Interplay between geometrical and electronic stability of neutral and anionic Cu-13 clusters: a first-principles study*  
European Physical Journal D, (58): 125-129 2010.

Zeng, X.; Gerken, M.; Beckers, H.; Willner, H.  
*Anomeric Effects in Sulfonyl Compounds: An Experimental and Computational Study of Fluorosulfonyl Azide, FSO<sub>2</sub>N<sub>3</sub>, and Trifluoromethylsulfonyl Azide, CF<sub>3</sub>SO<sub>2</sub>N<sub>3</sub>*  
Journal of Physical Chemistry A, (114): 7624-7630 2010.

Zeng, X.; Gerken, M.; Beckers, H.; Willner, H.

*Spectroscopic and Structural Studies of Difluorophosphoryl Azide F2P(O)N-3, Difluorophosphoryl Isocyanate F2P(O)NCO, and Difluorophosphoric Acid Anhydride, F-2(O)POP(O)F-2*  
Inorganic Chemistry, (49): 3002-3010 2010.

Zeng, X. Q.; Gerken, M.; Beckers, H.; Willner, H.  
*Spectroscopic and Structural Studies of Difluorophosphoryl Azide F2P(O)N-3, Difluorophosphoryl Isocyanate F2P(O)NCO, and Difluorophosphoric Acid Anhydride, F-2(O)POP(O)F-2*  
Inorganic Chemistry, (49): 3002-3010 2010.

Zervos, N.; Kocolouris, A.  
*Improper hydrogen-bonded cyclohexane C-H-ax center dot center dot center dot Y-ax contacts: experimental evidence from H-1 NMR spectroscopy of suitable axial cyclohexane models*  
Tetrahedron Letters, (51): 2453-2456 2010.

Zhai, H.-J.; Miao, C.-Q.; Li, S.-D.; Wang, L.-S.  
*On the Analogy of B-BO and B-Au Chemical Bonding in B11O- and B10Au- Clusters*  
Journal of Physical Chemistry A, (114): 12155-12161 2010.

Zhan, W.-S.; Pan, S.; Li, Y.-Z.; Chen, M.-D.  
*Molecular Design of D5 Analogues for Dye-Sensitized Solar Cells*  
Acta Physico-Chimica Sinica, (26): 1408-1416 2010.

Zhang, C. G.; Periyasamy, G.; Remacle, F.  
*Bonding Patterns of [Ag-2-Alanine](0, +/-) Hybrid Complexes and the Implementation of Molecular Logic Gates*  
International Journal of Quantum Chemistry, (110): 2237-2246 2010.

Zhang, G.; Gao, H.; Chen, D.  
*Chiral Discrimination in Hydrogen-Bonded Complexes of 2-Methyloxirane with Ethanol*  
Journal of Theoretical & Computational Chemistry, (9): 341-352 2010.

Zhang, G.; Qin, Y.; Zhang, H.; Shang, Y.; Sun, M.; Liu, B.; Li, Z.  
*Electronic Structure-Transport Property Relationships of Polyferrocenylene, Polyferrocenylacetylene, and Polyferrocenylsilane*  
Journal of Physical Chemistry C, (114): 9469-9477 2010.

Zhang, G.; Yuan, H.; Zhang, H.; Shang, Y.; Sun, M.; Liu, B.; Li, Z.  
*Theoretical studies of the transport property of oligosilane*  
Science China-Chemistry, (53): 2571-2580 2010.

Zhang, L.; Peslherbe, G. H.; Muchall, H. M.  
*A general measure of conjugation in biphenyls and their radical cations*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (88): 1175-1185 2010.

Zhang, L.; Yang, Y.; Xue, Y.; Fu, X.; An, Y.; Gao, G.  
*Experimental and theoretical investigation of reaction of aniline with dimethyl carbonate catalyzed by acid-base bifunctional ionic liquids*  
Catalysis Today, (158): 279-285 2010.

Zhang, M.; Zheng, Y.-P.; Jiang, X.-N.; Wang, C.-S.  
*Effect of Substituents on Hydrogen Bond Strength in N-H center dot center dot center dot O=C Hydrogen Bond Trimers*  
Acta Physico-Chimica Sinica, (26): 735-739 2010.

Zhang, R. B.; Eriksson, L. A.  
*Theoretical study on conformational preferences of ribose in 2-thiouridine-the role of the 2' OH group*  
Physical Chemistry Chemical Physics, (12): 3690-3697 2010.

Zhang, S. L.; Fu, Y.; Shang, R.; Guo, Q. X.; Liu, L.  
*Theoretical Analysis of Factors Controlling Pd-Catalyzed Decarboxylative Coupling of Carboxylic Acids with Olefins*  
Journal of the American Chemical Society, (132): 638-646 2010.

Zhang, S.-L.; Fu, Y.; Shang, R.; Guo, Q.-X.; Liu, L.  
*Theoretical Analysis of Factors Controlling Pd-Catalyzed Decarboxylative Coupling of Carboxylic Acids with Olefins*  
Journal of the American Chemical Society, (132): 638-646 2010.

Zhang, X.  
*Theoretical Study on Electronic Structure of (CNC)Fe\_2N(2) and Its N-2 Elimination Mechanism*  
International Journal of Quantum Chemistry, (110): 1880-1889 2010.

Zhang, X.; Zhang, P.; Song, J.; Xue, K.; Ban, Q.; Huang, J.  
*Synthesis, Crystal Structure, Theoretical Calculation, Specific Heat Capacity, and Thermodynamic Properties of 4-[(3-Ethoxyacetyl-2-thio)thiourea]-4'-[(3-ethoxyacetyl-2-thio)thiourea]diphenyloxide*  
Acta Chimica Sinica, (68): 1692-1698 2010.

Zhang, Y.; Chen, X.-Y.; Wang, H.-J.; Diao, K.-S.; Chen, J.-M.  
*DFT study on the structure and cation-anion interaction of amino acid ionic liquid of [C(3)mim](+)[Glu](-)*  
Journal of Molecular Structure-Theochem, (952): 16-24 2010.

Zhang, Y.; Liu, C.-Z.; Li, X.-J.; Wang, Z.-L.; Zhang, H.-T.; Miao, Z.-G.  
*Structures and energies of the radicals and anions generated from chlorpyrifos*  
Journal of Molecular Modeling, (16): 1369-1376 2010.

Zhang, Y.; Peng, S.; Li, X. J.; Zhang, D. X.  
*Structural stability, electronegativity and electronic property of endohedral TM@C-24 and exohedral TM-C-24 (TM = Sc, Y and La) metallofullerene complexes: Density-functional theory investigations*  
Journal of Molecular Structure-Theochem, (947): 16-21 2010.

Zhang, Y.; Vyas, S.; Hadad, C. M.; Platz, M. S.  
*An Ab Initio Study of the Ground and Excited State Chemistry of Phenyliazirine and Phenyliazomethane*

Journal of Physical Chemistry A, (114): 5902-5912 2010.

Zhang, Y.; Wasserman, A.

*Transferability of Atomic Properties in Molecular Partitioning: A Comparison*  
Journal of Chemical Theory and Computation, (6): 3312-3318 2010.

Zhang, Y.; Xu, W.; Sun, Q.; Zou, W.; Liu, W.

*Excited States of OsO<sub>4</sub>: A Comprehensive Time-Dependent Relativistic Density Functional Theory Study*  
Journal of Computational Chemistry, (31): 532-551 2010.

Zhao, Q.; Feng, D.; Hao, J.; Cal, Z.

*Chemical origin of contracted C-Cl bonds in the halogen-bonded complexes*  
Journal of Molecular Structure-Theochem, (958): 71-75 2010.

Zhao, S.; Ren, Y.; Ren, Y.; Wang, J.; Yin, W.

*Density functional study of CO binding on small AgnPdm clusters*  
Journal of Molecular Structure-Theochem, (955): 66-70 2010.

Zhao, S.; Ren, Y.; Ren, Y.; Wang, J.; Yin, W.

*Density Functional Study of Hydrogen Binding on Gold and Silver-Gold Clusters*  
Journal of Physical Chemistry A, (114): 4917-4923 2010.

Zheng, L.; He, H.; Yang, M.; Zeng, Q.; Yang, M.

*Identifying Tm@C-82 isomers with density functional theory calculations*  
Journal of Physics-Condensed Matter, (22) 2010.

Zheng, S.; Xiong, Y.; Wang, J.

*Theoretical studies on identity S(N)2 reactions of lithium halide and methyl halide: A microhydration model*  
Journal of Molecular Modeling, (16): 1931-1937 2010.

Zheng, W.-R.; Xu, J.-L.; Xiong, R.

*Density Functional Theory Study on N-O Bond Dissociation Enthalpies*  
Acta Physico-Chimica Sinica, (26): 2535-2542 2010.

Zheng, X.; Wang, X.; Shen, K.; Wang, N.; Peng, Y.

*Molecular Design of a "Molecular Syringe" Mimic for Metal Cations Using a 1,3-Alternate Calix[4]arene Cavity*  
Journal of Computational Chemistry, (31): 2143-2156 2010.

Zheng, X.; Wang, X.; Yi, S.; Wang, N.; Peng, Y.

*Density Functional Theory Study of Calix[4]arene-N-azacrown-5, Calix[4]arene-N-phenyl-azacrown-5, and Their Complexes with Alkali-Metal Cations: Na<sup>+</sup>, K<sup>+</sup>, and Rb<sup>+</sup>*  
Journal of Computational Chemistry, (31): 1458-1468 2010.

Zheng, X. Y.; Wang, X. Y.; Yi, S. F.; Wang, N. Q.; Peng, Y. M.

*Density Functional Theory Study of the Free and Tetraprotonated Spheroidal Macrotricyclic Ligands and the Complexes with Halide Anions: F-, Cl-, Br-*  
Journal of Computational Chemistry, (31): 871-881 2010.

Zhong, A.-G.; Huang, L.; Li, B.-L.; Jiang, H.-J.; Liu, S.-B.  
*Structure, Spectroscopy and Reactivity Properties of Helically Chiral Metal(II)-Bisdipyrin Complexes*  
Acta Physico-Chimica Sinica, (26): 2763-2771 2010.

Zhou, P.; Ren, Y.; Tian, F.; Zou, J.; Shang, Z.  
*Halogen-Ionic Bridges: Do They Exist in the Biomolecular World?*  
Journal of Chemical Theory and Computation, (6): 2225-2241 2010.

Zhou, S.; Chen, X.; Qian, C.  
*Quantum chemical modeling of the epoxidation with hydrogen peroxide catalyzed by Mn(III): Mechanistic insight*  
Chemical Physics Letters, (488): 44-49 2010.

Zhou, S. D.; Chen, X. Z.; Qian, C.  
*Quantum chemical modeling of the epoxidation with hydrogen peroxide catalyzed by Mn(III): Mechanistic insight*  
Chemical Physics Letters, (488): 44-49 2010.

Zhou, X.; Hrovat, D. A.; Borden, W. T.  
*Cyclooctatetraenes Tetrakis-Annelated with alpha-Dithio- or alpha-Diselenocarbonyl Groups: Diradicals Predicted To Have Ground States with 10 pi Electrons in the Eight-Membered Ring and Two-Center, Three-Electron, sigma Bonds between Two Pairs of Chalcogen Atoms*  
Journal of Physical Chemistry A, (114): 3683-3690 2010.

Zhou, Y.; Long, X.; Shu, Y.  
*Theoretical Study on the Azido-cyclization of 3,6-Di(azido)-1,2,4,5-tetrazine*  
Chinese Journal of Chemistry, (28): 2123-2129 2010.

Zhou, Z.-J.; Liu, H.-L.; Huang, X.-R.; Li, Q.-Z.; Sun, C.-C.  
*Effect of substitution and cooperativity on the Cl-F blue shift in single-electron halogen-bonded H3C center dot center dot center dot ClF complex*  
Molecular Physics, (108): 2021-2026 2010.

Zhu, Y.; Qi, D.; Zhang, L.; Wan, L.; Zhang, Y.; Jiang, J.  
*Structures and properties of novel 5,15-di[4-(5-acetylsulfanylpenyloxy)phenyl] porphyrin derivatives: Density functional theory calculations*  
Science China-Chemistry, (53): 2183-2192 2010.

Zierkiewicz, W.  
*Modelling of interactions between volatile anaesthetics (halothane, enflurane) and aromatic compounds, ab initio study*  
Chemical Physics, (373): 243-250 2010.

Zierkiewicz, W.; Michalska, D.; Zeegers-Huyskens, T.  
*Theoretical investigation of the conformation, acidity, basicity and hydrogen bonding ability of halogenated ethers*  
Physical Chemistry Chemical Physics, (12): 13681-13691 2010.

Zou, R.; Li, N.; Li, G.; Peng, B.; Luo, Q.; Li, Q.-S.  
*STRUCTURES AND STABILITIES B-9, B-9(+) and B-9(-) CLUSTERS*  
Revue Roumaine de Chimie, (55): 771-+ 2010.

Zubarev, D. Y.; Boldyrev, A. I.  
*Multiple Aromaticity, Multiple Antiaromaticity, and Conflicting Aromaticity in Planar Clusters*  
Nanoclusters: A Bridge across Disciplines: 219-267 2010.

Zubarev, D. Y.; Domin, D.; Lester, W. A.  
*Quantitative Characteristics of Qualitative Localized Bonding Patterns*  
Journal of Physical Chemistry A, (114): 3074-3079 2010.