

1. Magnetic and electronic properties of the nickel clusters Ni(n) ($n \leq 30$), Wei Song, Wen-Cai Lu, C. Z.Wang, K. M.Ho, *Comput. Theor. Chem.*, 978(1-3): 41-46, 2011
2. Fe-Fe adatom interaction and growth morphology on grapheme, Xiaojie Liu, C. Z.Wang, M.Hupalo, Wen-Cai Lu, P. A.Thiel, K. M.Ho, M. C.Tringides, *Phys. Rev. B*, 84(23): 235446, 2011
3. Theoretical mechanistic study of the reaction of the methylidyne radical with methylacetylene, Lili Zhang, Hui-ling Liu, Guang-Hui Yang, Xu-ri Huang, Yan Li, Yan-bo Sun, Chia-chung Sun, *J. Mol. Model.*, 17(12): 3173-3181, 2011
4. Theoretical Investigation on the Spectroscopic Properties of Cyclometallated Iridium (III) Complexes and the Deprotonation Influence on Them in Solution, Jian Wang, Bao-Hui Xia, Fu-Quan Bai, Lei Sun, Hong-Xing Zhang, *Int. J. Quantum Chem.*, 111(15): 4080-4090, 2011
5. Adsorption and dissociation of NO on Ir(100): A first-principles study, Chao-zheng He, Hui Wang, Peng Zhu, Jing-yao Liu, *J. Chem. Phys.*, 135(20): 204707, 2011
6. Visible-Light-Assisted HCHO Gas Sensing Based on Fe-Doped Flowerlike ZnO at Room Temperature, Lina Han, DeJun Wang, Yongchun Lu, Tengfei Jiang, Bingkun Liu, Yanhong Lin, *J. Phys. Chem. C*, 115(46): 22939-22944, 2011
7. Elucidation of the Methyl Transfer Mechanism Catalyzed by Chalcone O-Methyltransferase: A Density Functional Study, Feng-Chao Cui, Xiao-Liang Pan, Wei Liu, Jing-Yao Liu, *J. Comput. Chem.*, 32(14): 3068-3074, 2011
8. A Promising Approach to Obtain Excellent n-Type Organic Field-Effect Transistors: Introducing Pyrazine Ring, Xian-Kai Chen, Jing-Fu Guo, Lu-Yi Zou, Ai-Min Ren, Jian-Xun Fan, *J. Phys. Chem. C*, 115(43): 21416-21428, 2011
9. A high performance cobalt-doped ZnO visible light photocatalyst and its photogenerated charge transfer properties, Yongchun Lu, Yanhong Lin, Dejun Wang, Lingling Wang, Tengfeng Xie, Tengfei Jiang, *Nano Res.*, 4 (11): 1144-1152, 2011
10. Analysis of clinically relevant substrates of CYP2B6 enzyme by computational methods, Rui-Juan Niu, Qing-Chuan Zheng, Ji-Long Zhang, Hong-Xing Zhang, *J. Mol. Model.*, 17(11): 2839-2846, 2011
11. The influence of tether number and location on the self-assembly of polymer-tethered nanorods, Li Zhao, Xiang-Gui Xue, Zhong-Yuan Lu, Ze-Sheng Li, *J. Mol. Model.*, 17(11): 3005-3013, 2011
12. Efficient Blue-Emitting Ir(III) Complexes with Phosphine Carbanion-Based Ancillary Ligand: A DFT Study, Jian Wang, Fu-Quan Bai, Bao-Hui Xia, Hong-Xing Zhang, *J. Phys. Chem. A*, 115(42): 11689-11695, 2011
13. Graphite oxide-supported CaO catalysts for transesterification of soybean oil with methanol, Yanhong Zu, Jianyuan Tang, Wanchun Zhu, Min Zhang, Gang Liu, Yan Liu, Wenxiang Zhang, Mingjun Jia, *Bioresour. Technol.*, 102(19): 8939-8944, 2011
14. Dissipative Particle Dynamics Simulation Study On Controlling Molecular Weight Distribution In Emulsion Polymerization, Jing-Ming Zhang, Hui Li, Hong Liu,

- Chia-Chung Sun, *J. Theor. Comput. Chem.*, 10(5): 615-628, 2011
15. Mechanism and Kinetics Of The $\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3+\text{OH}$ Reaction: A Theoretical Study, Cong Hou, Cheng-Gang Ci, Tong-Yin Jin, Yong-Xia Wang, Jing-Yao Liu, *J. Theor. Comput. Chem.*, 10(5): 691-709, 2011
 16. Structure and Properties of Dual-Ti-Doped Single-Walled Carbon Nanotubes Within Density Functional Theory, Li-Li Yu, Sen Zhang, Qi Dong, Xian-Zhen Meng, Wei Quan Tian, *J. Comput. Theor. Nanosci.*, 8(9): 1811-1820, 2011
 17. Molecular Docking: A Powerful Approach for Structure-Based Drug Discovery, Xuan-Yu Meng, Hong-Xing Zhang, Mihaly Mezei, Meng Cui, *Curr. Comput.-Aided Drug Des.*, 7(2): 146-157, 2011
 18. DFT/TDDFT investigation of the electronic structures and optoelectronic properties of phosphorescent iridium (III) complexes with non-conjugated cyclometalated carbene ligands, Zai-Feng Xie, Fu-Quan Bai, Jian Wang, Hong-Xing Zhang, *Mol. Phys.*, 109(13): 1657-1675, 2011
 19. Evaporation- and surface-induced morphology of symmetric diblock copolymer thin films: a multibody dissipative particle dynamics study, Yan-Chun Li, Hong Liu, Xu-Ri Huang, Chia-Chung Sun, *Mol. Simul.*, 37(10): 875-883, 2011
 20. How dual bridging atoms tune structural and optoelectronic properties of ladder-type heterotetracenes?-a theoretical study, Xian-Kai Chen, Lu-Yi Zou, Ai-Min Ren, Jian-Xun Fan, *Phys. Chem. Chem. Phys.*, 13(43): 19490-19498, 2011
 21. Computational study of the one- and two-photon absorption properties of macrocyclic thiophene derivatives, Shuang Huang, Ai-Min Ren, Lu-Yi Zou, Yang Zhao, Jing-Fu Guo, Ji-Kang Feng, *Dyes Pigment.*, 91(2): 248-257, 2011
 22. Violating the general acidity-activity correlation: Computational evidence in a CpNa-modified HMCM-22 zeolite for ethene protonation, Ning He, Yi-hong Ding, *Microporous Mesoporous Mat.*, 144(1-3): 67-73, 2011
 23. Theoretical investigation of one- and two-photon spectra of pyrazobole chromophores, Xiao-Ting Liu, Lu-Yi Zou, Ai-Min Ren, Jing-Fu Guo, Ying Sun, Shuang Huang, Ji-Kang Feng, *Theor. Chem. Acc.*, 130(1): 37-50, 2011
 24. A theoretical study on magnesium ion-selective two-photon fluorescent probe based on benzo [h] chromene derivatives, Yang Zhao, Ai-Min Ren, Lu-Yi Zou, Jing-Fu Guo, Ji-Kang Feng, *Theor. Chem. Acc.*, 130(1): 61-68, 2011
 25. A DFT exploration of luminescent rhenium(I) tricarbonyl diimine complex with a triarylboron moiety and its F derivative, Jian Wang, Fu-Quan Bai, Bao-Hui Xia, Jie Chen, Hong-Xing Zhang, *J. Organomet. Chem.*, 696(18): 2943-2948, 2011
 26. Ab initio investigation on ion-associated species and association process in aqueous Na_2SO_4 and $\text{Na}_2\text{SO}_4/\text{MgSO}_4$ solutions, Hao Zhang, Song Wang, Chia-Chung Sun, *J. Chem. Phys.*, 135(8): 084309, 2011
 27. Shape Effect of Graphene Quantum Dots on Enhancing Second-Order Nonlinear Optical Response and Spin Multiplicity in NH_2 -GQD- NO_2 Systems, Zhong-Jun Zhou, Zhen-Bo Liu, Zhi-Ru Li, Xu-Ri Huang, Chia-Chung Sun, *J. Phys. Chem. C*, 115(33): 16282-16286, 2011
 28. Ab Initio and DFT Study of the Electronic Structures and Spectroscopic

- Properties of Pyrene Ligands and their Cyclometalated Complexes, Bao-Zhu Yang, Xin Zhou, Tao Liu, Fu-Quan Bai, Hong-Xing Zhang, *Int. J. Quantum Chem.*, 111 (10): 2258-2267, 2011
29. The Lithium-Orientation Effect on the Hyperpolarizability in the Short Zigzag-Edged Monolithiated Aza-Mobius Graphene Ribbon [2,7] Isomers, Yin-Feng Wang, Yi Wang, Zhi-Ru Li, Zhuo Li, Hong-Liang Xu, Chia-Chung Sun, *Int. J. Quantum Chem.*, 111 (10): 2406-2415, 2011
 30. Surface charge transfer properties of high-performance Ag-decorated ZnO photocatalysts, Yongchun Lu, Yanhong Lin, Dejun Wang, Lingling Wang, Tengfeng Xie, Tengfei Jiang, *J. Phys. D-Appl. Phys.*, 44(31): 315502, 2011
 31. Investigation of Photocatalytic Activities over Bi(2)WO(6)/ZnWO(4) Composite under UV Light and Its Photoinduced Charge Transfer Properties, Dongqing He, Lingling Wang, Dandan Xu, Jiali Zhai, Dejun Wang, Tengfeng Xie, *ACS Appl. Mater. Interfaces*, 3(8): 3167-3171, 2011
 32. Theoretical study on photophysical properties of 2,1,3-benzothiadiazole-based star-shaped molecules, Ying-Fang Liu, Xue-Feng Ren, Lu-Yi Zou, Ai-Min Ren, Ji-Kang Feng, Chia-Chung Sun, *Theor. Chem. Acc.*, 129(6): 833-845, 2011
 33. Structural, electronic, and optical properties of doubly ortho-linked quinoxaline/diphenylfluorene hybrids, Xue-Qin Ran, Ji-Kang Feng, Lu-Yi Zou, Ai-Min Ren, Chia-Chung Sun, *J. Phys. Org. Chem.*, 24(8): 646-656, 2011
 34. Synthesis of Zn-doped TiO(2) microspheres with enhanced photovoltaic performance and application for dye-sensitized solar cells, Yu Zhang, Lingling Wang, Bingkun Liu, Jiali Zhai, Haimei Fan, Dejun Wang, Yanhong Lin, Tengfeng Xie, *Electrochim. Acta*, 56(18): 6517-6523, 2011
 35. Alkali Metal Atom-Aromatic Ring: A Novel Interaction Mode Realizes Large First Hyperpolarizabilities of M@AR (M = Li, Na, and K, AR = Pyrrole, Indole, Thiophene, and Benzene), Guangtao Yu, Xu-Ri Huang, Wei Chen, Chia-Chung Sun, *J. Comput. Chem.*, 32 (9): 2005-2011, 2011
 36. Evolution of Lone Pair of Excess Electrons Inside Molecular Cages with the Deformation of the Cage in e(2)@C(60)F(60) Systems, Yin-Feng Wang, Wei Chen, Guang-Tao Yu, Zhi-Ru Li, Di Wu, Chia-Chung Sun , *J. Comput. Chem.*, 32 (9): 2012-2021, 2011
 37. Enhancement of Gas Sensing Properties of CdS Nanowire/ZnO Nanosphere Composite Materials at Room Temperature by Visible-Light Activation, Jiali Zhai, Lingling Wang, Dejun Wang, Haiyan Li, Yu Zhang, Dongqing He, Tengfeng Xie, *ACS Appl. Mater. Interfaces*, 3(7): 2253-2258, 2011
 38. Design of new benzothiadiazole-based linear and star molecules with different functional groups as solar cells materials: A theoretical approach, Lei Sun, Fu-Quan Bai, Zeng-Xia Zhao, Hong-Xing Zhang, *Sol. Energy Mater. Sol. Cells*, 95 (7): 1800-1810, 2011
 39. Theoretical investigation of charge injection and transport properties of novel organic semiconductor materials-cyclic oligothiophenes, Xian-Kai Chen, Lu-Yi Zou, Shuang Huang, Chun-Gang Min, Ai-Min Ren, Ji-Kang Feng, Chia-Chung Sun, *Org. Electron.*, 12 (7): 1198-1210, 2011

40. Charge injection and transfer tuning of a series of Pt complexes through oligothiophenes: A theoretical study, Xue-Feng Ren, Ai-Min Ren, Ying Sun, Jing-Fu Guo, Ji-Kang Feng, *J. Organomet. Chem.*, 696 (13): 2512-2518, 2011
41. Quantum Mechanical/Molecular Mechanical Molecular Dynamics and Free Energy Simulations of the Thiopurine S-Methyltransferase Reaction with 6-Mercaptopurine, Xiao-Liang Pan, Feng-Chao Cui, Jing-Yao Liu, *J. Phys. Chem. B*, 115 (24): 8033-8037, 2011
42. Hydrothermal synthesis and photoelectric properties of BiVO₄ with different morphologies: An efficient visible-light photocatalyst, Haimei Fan, Dejun Wang, Lingling Wang, Haiyan Li, Ping Wang, Tengfei Jiang, Tengfeng Xie, *Appl. Surf. Sci.*, 257(17): 7758-7762, 2011
43. Bonding and charge transfer by metal adatom adsorption on graphene, Xiaojie Liu, C. Z.Wang, Y. X.Yao,) W. C.Lu, M.Hupalo, M. C.Tringides, K. M.Ho, *Phys. Rev. B*, 83 (23 文献号: 235411, 2011
44. Theoretical study on the reaction of PH(+) with H₂O, Hongbo Xu, Huiling Liu, Jianchao Song, Yan Li, Yuhong Yang, Hao Tang,; Xuri Huang, *Comput. Theor. Chem.*, 966(1-3): 328-333, 2011
45. A comparative study of one- and two-photon absorption properties of pyrene and perylene diimide derivatives, Xiao-Ting Liu, Yang Zhao, Ai-Min Ren, Ji-Kang Feng, *J. Mol. Model.*, 17(6): 1413-1425, 2011
46. A comparative study on plate-like and flower-like ZnO nanocrystals surface photovoltage property and photocatalytic activity, Yongchun Lu, Lingling Wang, Dejun Wang, Tengfeng Xie, Liping Chen, Yanhong Lin, *Mater. Chem. Phys.*, 129(1-2): 281-287, 2011
47. Planar Tetracoordinate Carbon versus Planar Tetracoordinate Boron: The Case of CB₄ and Its Cation, Zhong-hua Cui, Maryel Contreras, Yi-Hong Ding, Gabriel Merino, *Journal of the American Chemical Society*, 133: 13228-13231, 2011
48. Energetic and fragmentation stability of water clusters (H₂O)_n, n=2-30, Xiaojie Liu, Wen-Cai Lu, C. Z.Wang, K.M. Ho, *Chem. Phys. Lett.*, 508(4-6): 270-275, 2011
49. An ab initio calculation study of silicon and carbon binary clusters C₇Si_n (n=1-7), Jing Zhang, Wen-Cai Lu, Qing-Jun Zang, Li-Zhen Zhao, C. Z.Wang, K. M.Ho, *J. Phys.-Condes. Matter*, 23(20): 205305, 2011
50. Effect of Heterojunction on the Behavior of Photogenerated Charges in Fe₃O₄@Fe₂O₃ Nanoparticle Photocatalysts, Xiao Wei, Tengfeng Xie, Linlin Peng, Wei Fu, Jiesheng Chen, Qian Gao, Guangyan Hong, Dejun Wang, *J. Phys. Chem. C*, 115(17): 8637-8642, 2011
51. Synthesis of Ordered Multivalent Mn-TiO₂ Nanospheres with Tunable Size: A High Performance Visible-Light Photocatalyst, Haiyan Li, Dejun Wang, Haimei Fan, Tengfei Jiang, Xinglin Li, Tengfeng Xie, *Nano Res.*, 4(5): 460-469, 2011
52. Supramolecular Assemblies Directed by Hydrogen Bonds and pi-pi Interactions and Based on N-Heterocyclic-Ligand-Modified beta-Octamolybdate - Structure and Catalytic Application in Olefin Epoxidation, Juan Du, Jiehui Yu, Jianyuan Tang, Jing Wang, Wenxiang Zhang, Werner R.Thiel, Mingjun Jia, *Eur. J. Inorg.*

- Chem., 15: 2361-2365, 2011
53. Theoretical design study on photophysical property of the organoboron quinolate derivatives, Lu-Yi Zou, Ai-Min Ren, Xue-Qin Ran, Xue-Feng Ren, Ji-Kang Feng, *Theor. Chem. Acc.*, 129(1): 63-71, 2011
 54. Theoretical Mechanistic Study on the Reaction of CN Radical with HNCN, Nan-Nan Wu, Chao-Zheng He, Xue-Mei Duan, Jing-Yao Liu, *J. Comput. Chem.*, 32(7): 1449-1455, 2011
 55. Direct Ab Initio Dynamics Study of Radical C(4)H ((X)over-tilde(2)Sigma(+)) + CH(4) Reaction, Rui-Ping Huo, Xiang Zhang, Xu-Ri Huang, Ji-Lai Li, Chia-Chung Sun, *J. Phys. Chem. A*, 115(15): 3576-3582, 2011
 56. Theoretical Studies on Mechanism and Kinetics of the Hydrogen-Abstraction Reaction of CF(3)CH(2)CHO with OH Radicals, Cheng-gang Ci, Hong-bo Yu, Su-qin Wan, Jing-yao Liu, Chia-Chung Sun, *Bull. Korean Chem. Soc.*, 32(4): 1187-1194, 2011
 57. The formation and decomposition of firefly dioxetanone, Chun-gang Min, Ai-min Ren, Xiao-na Li, Jing-fu Guo, Lu-yi Zou, Ying Sun, John D. Goddard, Chia-Chung Sun, *Chem. Phys. Lett.*, 506(4-6): 269-275, 2011
 58. Dissipative particle dynamics simulation study on complex structure transitions of vesicles formed by comb-like block copolymers, Hong Wang, Ying-Tao Liu, Hu-Jun Qian, Zhong-Yuan Lu, *Polymer*, 52(9): 2094-2101, 2011
 59. A Theoretical Survey on the Structures, Energetics, and Isomerization Pathways of the B(5)O Radical, Chang-Bin Shao, Lin Jin, Yi-Hong Ding, *J. Comput. Chem.*, 32(5): 771-777, 2011
 60. DIRECT DENSITY FUNCTIONAL THEORY DYNAMICS STUDY FOR THE CH(3)OCF(2)CF(2)OCH(3) + OH REACTION, Hong-Bo Yu, Feng-Chao Cui, Yong-Xia Wang, Hong-Xia Liu, Jing-Yao Liu, *J. Theor. Comput. Chem.*, 10(2): 231-244, 2011
 61. Theoretical study on the structures, isomerization, and stability of [Si, C, N, S] isomers, Ting-Ting Tao, Zhong-Jun Zhou, Yu-Hong Yang, Hui-Ling Liu, Xu-Ri Huang, Chia-Chung Sun, *Comput. Theor. Chem.*, 965(1): 123-130, 2011
 62. Theoretical study on the potential energy surface of the Si(2)PO system, Zhong-Jun Zhou, Xu-Ri Huang, Qing-Zhong Li, Chia-Chung Sun, *Comput. Theor. Chem.*, 965(1): 22-27, 2011
 63. Self-assembled monolayers of oligosilane on the silicon (001) surface: molecular dynamics simulations, Li Zhao, Xue-Mei Duan, Xiang-Gui Xue, Ming-Hui Li, Ze-Sheng Li, *J. Mol. Model.*, 17(4): 721-726, 2011
 64. 3D hierarchical flower-like TiO(2) nanostructure: morphology control and its photocatalytic property, Guohui Tian, Yajie Chen, Wei Zhou, Kai Pan, Chungui Tian, Xu-Ri Huang, Honggang Fu, *Crystengcomm*, 13(8): 2994-3000, 2011
 65. Amorphous mesoporous aluminophosphate as highly efficient heterogeneous catalysts for transesterification of diethyl carbonate with dimethyl carbonate, Jinghui Shi, Gang Liu, Zhiqiang Fan, Liying Nie, Zhihui Zhang, Wenxiang Zhang, Qisheng Huo, Wenfu Yan, Mingjun Jia, *Catal. Commun.*, 12(8): 721-725, 2011
 66. Theoretical Understanding of Ruthenium(II) Based Fluoride Sensor Derived from

- 4,5-Bis(benzimidazol-2-yl)imidazole (H₃ImBzim) and Bipyridine: Electronic Structure and Binding Nature, Jian Wang, Fu-Quan Bai, Bao-Hui Xia, Lei Sun, Hong-Xing Zhang, *J. Phys. Chem. A*, 115(10): 1985-1991, 2011
67. Ab Initio Investigation on a New Class of Binuclear Superalkali Cations M(2)Li(2k+1)(+) (F(2)Li(3)(+), O(2)Li(5)(+), N(2)Li(7)(+), and C(2)Li(9)(+)), Jing Tong, Ying Li, Di Wu, Zhi-Ru Li, Xu-Ri Huang, *J. Phys. Chem. A*, 115(10): 2041-2046, 2011
68. Electric Field-Driven Acid Base Chemistry: Proton Transfer from Acid (HCl) to Base (NH₃/H₂O), Zhong-Jun Zhou, Xiao-Ping Li, Zhen-Bo Liu, Zhi-Ru Li, Xu-Ri Huang, Chia-Chung Sun, *J. Phys. Chem. A*, 115(8): 1418-1422, 2011
69. Molecular dynamics studies of the 3D structure and planar ligand binding of a quadruplex dimer, Ming-Hui Li, Quan Luo, Xiang-Gui Xue, Ze-Sheng Li, *J. Mol. Model.*, 17(3): 515-526, 2011
70. DFT investigation on the reaction mechanism catalyzed by alpha-phosphomannomutase1 in protonated/deprotonated states, Hui-Ying Chu, Qing-Chuan Zheng, Xue Li, Yong-Shan Zhao, Ji-Long Zhang, Hong-Xing Zhang, *J. Mol. Model.*, 17(3): 577-585, 2011
71. Substitutional doping of BN nanotube by transition metal: A density functional theory simulation, Xi-Mao Li, Wei Quan Tian, Qi Dong, Xu-Ri Huang, Chia-Chung Sun, Lei Jiang, *Comput. Theor. Chem.*, 964(1-3): 199-206, 2011
72. Theoretical study of the low-lying electronic states of CCCF radical and its ions, Ming-Xing Song, Zeng-Xia Zhao, Wei Zhang, Fu-Quan Bai, Hong-Xing Zhang, Chia-Chung Sun, *Comput. Theor. Chem.*, 964(1-3): 277-282, 2011
73. Theoretical study on the mechanism of rearrangement reaction catalyzed by N(5)-carboxyaminoimidazole ribonucleotide mutase, Xue Li, Qing-Chuan Zheng, Ji-Long Hong-Xing Zhang, Zhang, *Comput. Theor. Chem.*, 964(1-3): 77-82, 2011
74. Complete oxidation of formaldehyde at ambient temperature over supported Pt/Fe₂O₃ catalysts prepared by colloid-deposition method, Nihong An, Qiushi Yu, Gang Liu, Suying Li, Mingjun Jia, Wenxiang Zhang, *J. Hazard. Mater.*, 186 (2-3): 1392-1397, 2011
75. Interface junction at anatase/rutile in mixed-phase TiO₂: Formation and photo-generated charge carriers properties, Xiaoru Zhang, Yanhong Lin, Dongqing He, Jianfu Zhang, Zhiyong Fan, Tengfeng Xie, *Chem. Phys. Lett.*, 504(1-3): 71-75, 2011
76. Direct ab initio dynamics study of the reaction of C(2)(A(3)Pi(u)) radical with C(2)H(6), Na Li, Rui-Ping Huo, Xiang Zhang, Xu-Ri Huang, Ji-Lai Li, Chia-Chung Sun, *Chem. Phys. Lett.*, 503(4-6): 210-214, 2011
77. Theoretical studies on structures and spectroscopic properties of a series of heteroleptic iridium complexes based on tridentate bis(benzimidazolyl)pyridine ligand, Yong Yang, Fu-Quan Bai, Hong-Xing Zhang, Xin Zhou, Chia-Chung Sun, *Comput. Theor. Chem.*, 963(2-3): 298-305, 2011
78. Carbon-rich C(9)Si(n) (n=1-5) clusters from ab initio calculations, Qiu-Xia Li, Wen-Cai Lu, Qing-Jun Zang, Li-Zhen Zhao, C. Z.Wang, K. M.Ho, *Comput. Theor. Chem.*, 963(2-3): 439-447, 2011

79. Theoretical improvement of the specific inhibitor of human carbonic anhydrase VII, Ji-Long Zhang, Qing-Chuan Zheng, Hong-Xing Zhang, *Comput. Biol. Chem.*, 35(1): 50-56, 2011
80. Exceptionally Large Second-Order Nonlinear Optical Response in Donor-Graphene Nanoribbon-Acceptor Systems, Zhong-Jun Zhou, Xiao-Ping Li, Fang Ma, Zhen-Bo Liu, Zhi-Ru Li, Xu-Ri Huang, Chia-Chung Sun, *Chem.-Eur. J.*, 17(8): 2414-2419, 2011
81. Time-Dependent Density Functional Theory Study on the Absorption Spectrum of Coumarin 102 and Its Hydrogen-Bonded Complexes, Wenwei Zhao, Yihong Ding, Qiying Xia, *J. Comput. Chem.*, 32(3): 545-553, 2011
82. Phase diagram of spherical particles interacted with harmonic repulsions, You-Liang Zhu, Zhong-Yuan Lu, *J. Chem. Phys.*, 134 (4): 044903, 2011
83. Reaction mechanism of isoflavone O-methyltransferase: A theoretical investigation, Feng-Chao Cui, Xiao-Liang Pan, Jing-Yao Liu, *Chem. Phys. Lett.*, 501(4-6): 502-507, 2011
84. On the viability of cyclometalated Ru(II) complexes as dyes in DSSC regulated by COOH group, a DFT study, Jian Wang, Fu-Quan Bai, Bao-Hui Xia, Lu Feng, Hong-Xing Zhang, Qing-Jiang Pan, *Phys. Chem. Chem. Phys.*, 13 (6): 2206-2213, 2011
85. Can isocyanogen azide exist?, Si-meng Gao, Li-juan Fu, Zhong-hua Cui, Yi-hong Ding, *Mol. Phys.*, 109 (4): 589-601, 2011
86. Direct evidence for the effect of lateral hydrogen bonding on the smectic phase, Haitao Wang, Binglian Bai, Fu-Quan Bai, Dongmei Pang, Xia Ran, Chengxiao Zhao, Hong-Xing Zhang, Min Li, *Liq. Cryst.*, 38(6): 767-774, 2011
87. Molecular dynamics simulation study on the isomerization and molecular orientation of liquid crystals formed by azobenzene and (1-cyclohexenyl)phenyldiazene, Xiang-Gui Xue, Li Zhao, Zhong-Yuan Lu, Ming-Hui Li, Ze-Sheng Li, *Phys. Chem. Chem. Phys.*, 13(25): 11951-11957, 2011
88. What is the role of defects in single-walled carbon nanotubes for nonlinear optical property?, Zhen-Bo Liu, Zhong-Jun Zhou, Zhi-Ru Li, Qing-Zhong Li, Feng-Yan Jia, Jian-Bo Cheng, Chia-Chung Sun, *J. Mater. Chem.*, 21(24): 8905-8910, 2011
89. Self-assembled 3D hierarchical clew-like Bi₂WO₆ microspheres: Synthesis, photo-induced charges transfer properties, and photocatalytic activities, Dongqing He, Lingling Wang, Haiyan Li, Tianyi Yan, Dejun Wang, Tengfeng Xie, *Crystengcomm*, 13(12): 4053-4059, 2011
90. NXAl₃(⁺) (X = N, P, As): penta-atomic planar tetracoordinate nitrogen with N-X multiple bonding, Zhong-hua Cui, Yi-hong Ding, *Phys. Chem. Chem. Phys.*, 13(13):5960-5966, 2011
91. Low-lying electronic states of HNCS and its ions: a CASSCF/CASPT2 study, Tao Liu, Zeng-Xia Zhao, Ming-Xing Song, Hong-Xing Zhang, Chia-Chung Sun, *Theor. Chem. Acc.*, 128 (2): 215-222, 2011
92. Hydrogen storage capacity of Ti substitution-doped pyracylene: Density

- functional theory investigations, Sen Zhang, Xian-Zhen Meng, Li-Li Yu, Qi Dong, Wei-Quan Tian, *Int. J. Hydrog. Energy*, 36(1): 606-615, 2011
93. Dihydrogen bond in $C(2)H(4-n)Cl(n) \dots NaH$ ($n=0, 1, 2, 3$) complexes: ab initio, AIM and NBO studies, Lu Feng, Fu-Quan Bai, Yang Wu, Hong-Xing Zhang, *Mol. Phys.*, 109 (5):645-653, 2011
 94. Theoretical study of one- and two-photon absorption properties of pyrene derivatives, Yang Zhao, Jing-Fu Guo, Ai-Min Ren, Ji-Kang Feng, *Theor. Chem. Acc.*, 128 (2):265-274, 2011
 95. Beryllium and boron decoration forms planar tetracoordinate carbon strips at the edge of graphene nanoribbons, Bo Xiao, Yi-hong Ding, Chia-chung Sun, *Phys. Chem. Chem. Phys.*, 13 (7): 2732-2737, 2011
 96. A single-site anisotropic soft-core model for the study of phase behavior of soft rodlike particles, Li ZhanWei; Liu YuHua; Liu YingTao; Lu ZhongYuan, *Sci. China-Chem.*, 54(9): 1474-1483, 2011
 97. Mechanism and Kinetics of the $CH(3)OCF(2)CF(2)OCH(3)+Cl$ Reaction, Cui Feng-Chao; Yu Hong-Bo; Wang Qin; Ye Wan-Li; Liu Jing-Yao, *Acta Phys.-Chim. Sin.*, 27(2): 337-342, 2011
 98. Multi-scale Molecular Simulations Study on the Gating Mechanism in a Pentameric Ligand-gated Ion Channel from *Gloeobacter Violaceus*, Yu Hui; Li Zhuo; Zhao Xi; Huang Xuri, *Acta Chim. Sin.*, 69(14): 1639-1644, 2011
 99. Theoretical Studies on Photodissociation Mechanism of Glycolaldehyde, Ci Cheng-Gang; Duan Xue-Mei; Liu Jing-Yao; Sun Chia-Chung, *Chem. J. Chin. Univ.-Chin.*, 32 (7): 1588-1593, 2011
 100. Structures and Spectroscopic Properties of Highly Efficient Luminescence Material Cationic $[(C)_{over-capN}(2)IrL](+)$ Complexes, Zhang Jian-Po; Jin Li; Zhang Hong-Xing; Bai Fu-Quan, *Chem. J. Chin. Univ.-Chin.*, 32(12): 2885-2890, 2011
 101. Theoretical Investigation of the Reaction Mechanism of Cypridina Luciferin Analogues, Sun Ying; Ren Ai-Min; Li Zuo-Sheng; Min Chun-Gang; Ren Xue-Feng; Feng Ji-Kang, *Chem. J. Chin. Univ.-Chin.*, 32(11): 2586-2592, 2011
 102. Nondriven Polymer Translocation Through a Nanopore: Scaling for Translocation Time with Chain Length, Li Hui; Zhang Jing; Liu Hong; Sun Chia-chung, *Chem. Res. Chin. Univ.*, 27(6): 1023-1026, 2011
 103. DFT/TDDFT Studies on the Electronic Structures and Spectral Properties of Carbazole-based Blue Light-emitting Dendrimers, Li Leijiao; Feng Jikang; Ren Aimin; Sun Chiachung, *Chin. J. Chem.*, 29(11): 2263-2270, 2011
 104. Effect of Explicit Water Molecules on the Color-Tuning Mechanism of the Firefly, Min Chungang; Zou Luyi; Sun Ying; Guo Jingfu; Ren Ai-min; Goddard, John D., *Chin. J. Chem.*, 29(11): 2301-2307, 2011,
 105. Dissipative Particle Dynamics Simulation of Association Reaction in Telechelic Polymers, Li Hui; Zhang Jing; Liu Hong; Sun Chia-Chung, *Chem. J. Chin. Univ.-Chin.*, 32(10): 2410-2414, 2011
 106. Multibody Dissipative Particle Dynamics Study of the Composition Effect on the Morphology of Block Copolymer Thin Film, Li Yan-Chun; Liu Hong; Huang

- Xu-Ri; Sun Chia-Chung, *Chem. J. Chin. Univ.-Chin.*, 32(10): 2421-2426, 2011
107. Theoretical Study on the Two-Photon Absorption Properties of Pyrazole Aluminum Compounds, Liu Xiao-Ting; Guo Jing-Fu; An Di; Wang Dan; Ren Ai-Min; Feng Ji-Kang, *Acta Phys.-Chim. Sin.*, 27(10): 2303-2310, 2011
108. DFT Study on the Copolymerization Mechanism of Ethylene with Cyclopentadiene by the Titanium Complexes Bearing Two beta-Enaminoketonato Ligands, Wang Yongxia; Duan Xuemei; Wang Qin; Li Yuesheng; Liu Jingyao, *Acta Chim. Sin.*, 69(18): 2085-2091, 2011
109. Dissipative Particle Dynamics Study of Homopolymer Adsorb on Micelle in Non-equilibrium State, Li Yan-Chun; Liu Hong; Huang Xu-Ri; Sun Chia-Chung, *Chem. J. Chin. Univ.-Chin.*, 32(8): 1845-1848, 2011
110. Using Raman Spectroscopy and ab initio Calculations to Investigate Intermolecular Hydrogen Bonds in Binary Mixture (Tetrahydrofuran plus Water), Wu Nan-nan; Ouyang Shun-li; Li Zuo-wei; Liu Jing-yao; Gao Shu-qin, *Chem. Res. Chin. Univ.*, 27(4): 693-696, 2011
111. Theoretical Investigation of Chemically Enhanced Mechanism of SERS Spectroscopy for Ag/MPH/TiO(2) System, Sun Lei; Bai Fu-Quan; Zhang Hong-Xing, *Acta Phys.-Chim. Sin.*, 27(6): 1335-1340, 2011
112. Lithium Salt of NH(2)-substituted Graphene Nanoribbon with Twofold Donor-acceptor Framework: Large Nonlinear Optical Property, Zhou Zhong-jun; Li Zhi-ru; Huang Xu-ri; Sun Chia-chung, *Chem. Res. Chin. Univ.*, 27(3):512-515, 2011
113. Influence of Solid-liquid Interaction and Temperature on the Dynamic Dewetting of a Thin Polymer Film: A Molecular Dynamics Study, Zhao Li; Xue Xiang-gui; Lu Zhong-yuan, *Chem. Res. Chin. Univ.*, 27(2):324-328, 2011
114. Imitating trumpet shells: Mobius container molecules, Ma Fang; Wang FangFang; Li ZhiRu; Wu Di; Li ZeSheng; Gu FengLong, *Sci. China-Chem.*, 54(3):454-460, 2011
115. Assessing the Credibility of VDAC Structure with Molecular Dynamics Simulation Approach, Sun Tie-Dong; Zhao Xi; Huang Xu-Ri, *Chem. J. Chin. Univ.-Chin.*, 32(2):327-331, 2011
116. Multi-scale Simulation Model on the Co-polymerization Between Ethylene and Propylene, Liu Yu-Hua; Liu Hong; Liu Jing-Yao; Lu Zhong-Yuan, *Chem. J. Chin. Univ.-Chin.*, 32(2):332-338, 2011
117. Chiral Selectivity of Arginase I, Li Shuai; Li Zhao-Long; Hu Yu-Lin; Gao Xue-Feng; Huang Xu-Ri, *Chem. J. Chin. Univ.-Chin.*, 32(6): 1339-1342, 2011