

1. Nonlinear optical properties for a class of hexa-peri-hexabenzocoronene chromophores: a computational investigation, Liu, Xiao-Ting; Guo, Jing-Fu; Ren, Ai-Min; Huang, Shuang; Feng, Ji-Kang, *Dalton Trans.*, 41(40): 12416-12427, 2012
2. Theoretical insight into linear optical and two-photon absorption properties for a series of N-arylpyrrole-based dyes, Liu, Xiao-Ting; Guo, Jing-Fu; Ren, Ai-Min; Xu, Zhong; Huang, Shuang; Feng, Ji-Kang, *Org. Biomol. Chem.*, 10(37): 7527-7535, 2012
3. Mechanism of benzene hydroxylation by high-valent bare Fe-IV=O²⁺: explicit electronic structure analysis, Li, Ji-Lai; Zhang, Xiang; Huang, Xu-Ri, *Phys. Chem. Chem. Phys.*, 14(1): 246-256, 2012
4. Computational study of the electronic structures, UV-Vis spectra and static second-order nonlinear optical susceptibilities of macrocyclic thiophene derivatives, Huang, Shuang; Ren, Ai-Min; Zou, Lu-Yi; Zhao, Yang; Guo, Jing-Fu; Feng, Ji-Kang, *J. Mol. Model.*, 18(1): 393-404, 2012
5. Theoretical Prediction of One- and Two-Photon Absorption Properties of N-Annulated Quaterrylenes as Near-Infrared Chromophores, Liu, Xiao-Ting; Guo, Jing-Fu; Ren, Ai-Min; Huang, Shuang; Feng, Ji-Kang, *J. Org. Chem.*, 77(1): 585-597, 2012
6. Free energy and scalings for polymer translocation through a nanopore: A molecular dynamics simulation study combined with milestoning, Xue, Xiang-Gui; Zhao, Li; Lu, Zhong-Yuan; Li, Ze-Sheng, *Phys. Lett. A*, 376(4): 290-292, 2012
7. From Molecules to Materials: Molecular and Crystal Engineering Design of Organic Optoelectronic Functional Materials for High Carrier Mobility, Chang, Ying-fei; Lu, Zhong-yuan; An, Li-jia; Zhang, Jing-ping, *J. Phys. Chem. C*, 116(1): 1195-1199, 2012
8. Effect of BiVO₄ Crystalline Phases on the Photoinduced Carriers Behavior and Photocatalytic Activity, Fan, Haimei; Jiang, Tengfei; Li, Haiyan; Wang, Dejun; Wang, Lingling; Zhai, Jiali; He, Dongqing; Wang, Ping; Xie, Tengfeng, *J. Phys. Chem. C*, 116(3) 特刊: SI: 2425-2430, 2012
9. Direct ab initio dynamics study of the reaction of C-2(A(3)Pi(u)) with CH₄, Huo, Rui-Ping; Huang, Xu-Ri; Li, Ji-Lai; Zhang, Xiang; Li, Na; Sun, Chia-Chung, *Int. J. Quantum Chem.*, 112(4): 1078-1085, 2012
10. Double icosahedron-based motif of Nin (n=20-30), Song, Wei; Lu, Wen-Cai; Zang, Qing-Jun; Wang, C. Z.; Ho, K. M., *Int. J. Quantum Chem.*, 112(6): 1717-1724, 2012
11. Mechanism Insights of Ethane C-H Bond Activations by Bare [Fe-III=O](⁺): Explicit Electronic Structure Analysis, Sun, Xiao-Li; Huang, Xu-Ri; Li, Ji-Lai; Huo, Rui-Ping; Sun, Chia-Chung, *J. Phys. Chem. A*, 116(5): 1475-1485, 2012
12. Toward highly fluorescence and ultralow-threshold amplified spontaneous emission in ordered solid state from twin-tapered bi-1,3,4-oxadiazole derivatives, Qu, Songnan; Wang, Haitao; Zhu, Wanbin; Luo, Jinsong; Fan, Yi; Song, Liwei; Zhang, Hong-Xing; Liu, Xingyuan, *J. Mater. Chem.*, 22(9): 3875-3881, 2012

13. Mesoporous SBA-15 modified with manganese pyrazolylpyridine complexes for the catalytic epoxidation of terminal alkenes, Tang, Jianyuan; Zu, Yanhong; Huo, Weitao; Wang, Lei; Wang, Jing; Jia, Mingjun; Zhang, Wenxiang; Thiel, Werner R., *J. Mol. Catal. A-Chem.*, 355: 201-209, 2012
14. Fine tuning of the one- and two-photon absorption properties of macrocyclic thiophene-based derivatives, Huang, Shuang; Zou, Lu-Yi; Ren, Ai-Min; Zhao, Yang; Liu, Xiao-Ting; Guo, Jing-Fu; Feng, Ji-Kang, *Dyes Pigment.*, 93(1-3): 1519-1531, 2012
15. Vapor phase ortho-selective alkylation of phenol with methanol over silica-manganese mixed oxide catalysts, Wang, Yanli; Song, Yingying; Huo, Weitao; Jia, Mingjun; Jing, Xiaoyan; Yang, Piaoping; Yang, Zhi; Liu, Gang; Zhang, Wenxiang, *Chem. Eng. J.*, 181): 630-635, 2012
16. An efficient strategy for designing n-type organic semiconductor materials-introducing a six-membered imide ring into aromatic diimides, Chen, Xian-Kai; Zou, Lu-Yi; Guo, Jing-Fu; Ren, Ai-Min, *J. Mater. Chem.*, 22(13): 6471-6484, 2012
17. Tuning the band gaps and work functions via topology and carbon concentration: a first-principles investigation of C-x(BN)(y) compounds, Xie, Ying; Yu, Haitao; Zhang, Hongxing; Fu, Honggang, *Phys. Chem. Chem. Phys.*, 14(13): 4391-4397, 2012
18. Graphitic Carbon Nanocapsules: Scaled Preparation, Formation Mechanism, and Use as an Excellent Support for Methanol Electro-oxidation, Wang, Lei; Tian, Chungui; Zhang, Hongxing; Fu, Honggang, *Eur. J. Inorg. Chem.*, 6: 961-968, 2012
19. A theoretical study of the ring size effect on one- and two-photon absorption properties of macrocyclic thiophene derivatives, Huang, Shuang; Zou, Lu-Yi; Ren, Ai-Min; Guo, Jing-Fu; Liu, Xiao-Ting; Feng, Ji-Kang, *New J. Chem.*, 36(4): 947-953, 2012
20. UV-illumination room-temperature gas sensing activity of carbon-doped ZnO microspheres, Zhai, Jiali; Wang, Lingling; Wang, Dejun; Lin, Yanhong; He, Dongqing; Xie, Tengfeng, *Sens. Actuator B-Chem.*, 161(1): 292-297, 2012
21. Intercage Electron Transfer Driven by Electric Field in Robin-Day-Type Molecules, Wang, Yin-Feng; Li, Ying; Zhou, Zhong-Jun; Li, Zhi-Ru; Wu, Di; Huang, Jianguo; Gu, Feng Long, *ChemPhysChem*, 13(3): 756-761, 2012
22. Magnetic nanoparticles/graphitic carbon nanostructures composites: Excellent magnetic separable adsorbents for precious metals from aqueous solutions, Wang, Lei; Tian, Chungui; Mu, Guang; Sun, Li; Zhang, Hongxing; Fu, Honggang, *Mater. Res. Bull.*, 47(3): 646-654, 2012
23. Geometries and stabilities of Ag-n(nu) (nu = +/- 1, 0; n=21-29) clusters, Yan, Shu-Yao; Zhang, Wei; Zhao, Zeng-Xia; Lu, Wen-Cai; Zhang, Hong-Xing, *Theor. Chem. Acc.*, 131(3) 文献号: 1200, 2012
24. Electrochemical oxidation of aqueous phenol at low concentration using Ti/BDD electrode, Sun, Jianrui; Lu, Haiyan; Lin, Haibo; Du, Lili; Huang, Weimin; Li, Hongdong; Cui, Tian, *Sep. Purif. Technol.*, 88: 116-120, 2012

25. Positioning of Ftz-F1 Domain Affects on the Activity of Human LRH-1: Molecular Dynamics Study on Human LRH-1-DNA Complexes, Li, Shuai; Wu, Lei; Yu, Hui; Gao, Xuefeng; Li, Zhengqiang; Zhao, Xi; Huang, Xu-Ri, *J. Theor. Comput. Chem.*, 11(2): 329-359, 2012
26. The interaction between superalkalis (M₃O, M = Na, K) and a C₂₀F₂₀ cage forming superalkali electride salt molecules with excess electrons inside the C₂₀F₂₀ cage: dramatic superalkali effect on the nonlinear optical property, Wang, Jia-Jun; Zhou, Zhong-Jun; Bai, Yang; Liu, Zhen-Bo; Li, Ying; Wu, Di; Chen, Wei; Li, Zhi-Ru; Sun, Chia-Chung, *J. Mater. Chem.*, 22(19): 9652-9657, 2012
27. Photoelectric properties of ZnO/Ag₂S heterostructure and its photoelectric ethanol sensing characteristics, Zhang, Yu Liu, Bingkun; Wang, Dejun; Lin, Yanhong; Xie, Tengfeng; Zhai, Jiali, *Mater. Chem. Phys.*, 133(2-3): 834-838, 2012
28. Theoretical investigation of the two-photon absorption properties of 3,6-bis(4-vinylpyridinium) carbazole derivatives-new biological fluorescent probes, Sun, Ying; Zhao, Yang; Liu, Xiao-Ting; Ren, Ai-Min; Feng, Ji-Kang; Yu, Xiao-Qiang, *J. Mol. Model.*, 18(6): 2357-2367, 2012
29. Theoretical Study on Polynuclear Superalkali Cations with Various Functional Groups as the Central Core, Tong, Jing; Li, Ying; Wu, Di; Wu, Zhi-Jian, *Inorg. Chem.*, 51(11): 6081-6088, 2012
30. Theoretical studies on spectroscopic properties of ruthenium sensitizers absorbed to TiO₂ film surface with connection mode for DSSC, Chen, Jie; Bai, Fu-Quan; Wang, Jian; Hao, Li; Xie, Zai-Feng; Pan, Qing-Jiang; Zhang, Hong-Xing, *Dyes Pigment.*, 94(3): 459-468, 2012
31. Self-assembly of amphiphilic patchy particles with different cross-linking densities, Zhang, Jing; Lu, Zhong-Yuan; Sun, Zhao-Yan, *Soft Matter*, 8(26): 7073-7080, 2012
32. A critical theoretical study on linear and nonlinear optical properties of macrocyclic thiophene derivatives with different connecting pi-conjugated bridge and ring size, Huang, Shuang; Ren, Ai-Min; Guo, Jing-Fu; Liu, Xiao-Ting; Feng, Ji-Kang, *Polymer*, 53(14): 2991-3000, 2012
33. Molecular Dynamics Simulations Suggest Ligand's Binding to Nicotinamidase/Pyrazinamidase, Zhang, Ji-Long; Zheng, Qing-Chuan; Li, Zheng-Qiang; Zhang, Hong-Xing, *PLoS One*, 7(6) 文献号: e39546, 2012
34. DFT and TD-DFT study on the electronic structures and phosphorescent properties of 6-phenyl-2,2'-bipyridine tridentate iridium(III) complexes and their isomer, Bai, Fu-Quan; Wang, Jian; Xia, Bao-Hui; Pan, Qing-Jiang; Zhang, Hong-Xing, *Dalton Trans.*, 41(27): 8441-8446, 2012
35. Quantum Mechanical Design and Structures of Hexanuclear Sandwich Complex and Its Multidecker Sandwich Clusters (Li₆)(n)([18] Annulene)(n+1) (n=1-3), Wang, Shu-Jian; Li, Ying; Wu, Di; Wang, Yin-Feng; Li, Zhi-Ru, *J. Phys. Chem. A*, 116(36): 9189-9196, 2012
36. Transesterification of dimethyl oxalate with phenol over nitrogen-doped nanoporous carbon materials, Yuan, Xiaoling; Zhang, Min; Chen, Xiaodong; An,

- Nihong; Liu, Gang; Liu, Yan; Zhang, Wenxiang; Yan, Wenfu; Jia, Mingjun, *Appl. Catal. A-Gen.*, 439: 149-155, 2012
37. Direct ab initio dynamics study of rate constants and kinetic isotope effects for C-2(A(3)Pi(u)) + CH₃OH reaction, Huo, Rui-Ping; Zhang, Xiang; Huang, Xu-Ri; Li, Ji-Lai; Sun, Chia-Chung, *Mol. Phys.*, 110(18): 2205-2217, 2012
 38. Photoinduced Charge Transfer Properties and Photocatalytic Activity in Bi₂O₃/BaTiO₃ Composite Photocatalyst, Fan, Haimei; Li, Haiyan; Liu, Bingkun; Lu, Yongchun; Xie, Tengfeng; Wang, Dejun, *ACS Appl. Mater. Interfaces*, 4(9): 4853-4857, 2012
 39. Theoretical studies on the electronic structures and optical properties of the thiophene oligomer containing 2-(trifluoromethyl) thieno [3, 4-b] thiophene moiety and the CF₃ end-caps, Wei, Wei; Bai, Fu-Quan; Xia, Bao-Hui; Zhang, Hong-Xing, *J. Polym. Res.*, 19(10) 文献号: 9972, 2012
 40. Theoretical Analysis on Molecular Magnetic Properties of N-Confused Porphyrins and Its Derivatives, Wei, Wei; Bai, Fu-Quan; Xia, Bao-Hui; Zhang, Hong-Xing, *Bull. Korean Chem. Soc.*, 33(9): 2937-2942, 2012
 41. Influence of Grafting Surface Curvature on Chain Polydispersity and Molecular Weight in Concave Surface-Initiated Polymerization, Liu, Hong; Zhu, You-Liang; Zhang, Jing; Lu, Zhong-Yuan; Sun, Zhao-Yan, *ACS Macro Lett.*, 1(11): 1249-1253, 2012
 42. Decomposition of Methanol on Clean and Oxygen-Predosed V(100): A First-Principles Study, Wang, Hui; He, Chao-zheng; Huai, Li-yuan; Tao, Fu-ming; Liu, Jing-yao, *J. Phys. Chem. C*, 116(48): 25344-25353, 2012
 43. Specific binding structures of dendrimers on lipid bilayer membranes, Wang, Yong-Lei; Lu, Zhong-Yuan; Laaksonen, Aatto, *Phys. Chem. Chem. Phys.*, 14(23): 8348-8359, 2012
 44. Structural Characteristics and Large Non-Linear Optical Responses of New Alkaline Earth-Based Alkalides, Fan, Li-Tao; Li, Ying; Wu, Di; Li, Zhi-Ru; Sun Chia-Chung, *Aust. J. Chem.*, 65(2): 138-144, 2012
 45. Insights into the thermal stabilization and conformational transitions of DNA by hyperthermophile protein Sso7d: molecular dynamics simulations and MM-PBSA analysis, Chen, Lin; Zheng, Qing-Chuan; Yu, Li-Ying; Chu, Wen-Ting; Zhang, Ji-Long; Xue, Qiao; Zhang, Hong-Xing; Sun, Chia-Chung, *J. Biomol. Struct. Dyn.*, 30(6): 716-727, 2012
 46. The effect of the axial ligand on distinct reaction tunneling for methane hydroxylation by nonheme iron(IV)-oxo complexes, Tang, Hao; Guan, Jia; Zhang, Lili; Liu, Huiling; Huang, Xuri, *Phys. Chem. Chem. Phys.*, 14(37): 12863-12874, 2012
 47. Evolution of the structural and electronic properties of beryllium-doped aluminum clusters: comparison with neutral and cationic aluminum clusters, Sun, Wei-Ming; Li, Ying; Wu, Di; Li, Zhi-Ru, *Phys. Chem. Chem. Phys.*, 14(47): 16467-16475, 2012
 48. Structural properties and nonlinear optical responses of superatom compounds BF₄-M (M = Li, FLi₂, OLi₃, NLi₄), Yang, Hui; Li, Ying; Wu, Di; Li, Zhi-ru, *Int.*

- J. Quantum Chem., 112(3): 770-778, 2012
49. Quantum chemical modeling of 1,1-proton transfer reaction catalyzed by a cofactor-independent alpha-methylacyl-CoA racemase, Li, Xue; Zheng, Qing-Chuan; Zhang, Hong-Xing, Int. J. Quantum Chem., 112(2): 619-624, 2012
 50. Structural and energetic exploration of a boron-rich sulfide cluster B₆S, Tang, Xiao-Yu; Cui, Zhong-Hua; Shao, Chang-Bin; Ding, Yi-Hong, Int. J. Quantum Chem., 112(5): 1299-1306, 2012
 51. Theoretical investigations on electronic structures and photophysical properties of novel bridged triphenylamine derivatives, Zhang, Zi-Long; Zou, Lu-Yi; Ren, Ai-Min; Min, Chun-Gang; Sun, Ying; Liu, Ying-Fang, Int. J. Quantum Chem., 112(5): 1473-1490, 2012
 52. A CASSCF/CASPT2 study on the low-lying electronic states of the CH₃SS and its cation, Song, Ming-Xing; Zhao, Zeng-Xia; Zhang, Wei; Bai, Fu-Quan; Zhang, Hong-Xing; Sun, Chia-Chung, Int. J. Quantum Chem., 112(6): 1537-1546, 2012
 53. Theoretical study on the ion-molecule reaction of NH⁺ with CH₂O, Song, Jian-Chao; Liu, Hui-Ling; Zhou, Zhong-Jun; Huang, Xu-Ri, Int. J. Quantum Chem., 112(6): 1654-1666, 2012
 54. Theoretical study on the electronic structures and photophysical properties of a series of dithienylbenzothiazole derivatives, Li, Yan; Zou, Lu-Yi; Ren, Ai-Min; Feng, Ji-Kang, Comput. Theor. Chem., 981: 14-24, 2012
 55. Theoretical study on optoelectronic properties of fluorene derivatives with pyrene-functional groups: effect of the heteroatoms and pyrene' substituting position, Chen, Xian-Kai; Zou, Lu-Yi; Ren, Ai-Min; Fan, Jian-Xun, Mol. Phys., 110(3): 163-172, 2012
 56. Theoretical study for the CH₃OCF₂CF₂OCHO + Cl reaction, Jin, Tong-yin; Yu, Hong-bo; Ci, Cheng-gang; Liu, Jing-yao, Theor. Chem. Acc., 131(2) 文献号: 1119
 57. Brownian dynamics simulation study on the self-assembly of incompatible star-like block copolymers in dilute solution, Li, Bin; Zhu, You-Liang; Liu, Hong; Lu, Lu, Zhong-Yuan, Phys. Chem. Chem. Phys., 14(14): 4964-4970, 2012
 58. Role of Hydrocarbon Radicals CH_x (x=1, 2, 3) in Graphene Growth: A Theoretical Perspective, Wang, Chong; Xiao, Bo; Ding, Yi-hong, ChemPhysChem, 13(3): 774-779, 2012
 59. Theoretical studies of the structural, electronic and optical properties of carbazole-based compounds, Li, Lei-Jiao; Bai, Fu-Quan; Zhang, Hong-Xing, J. Phys. Org. Chem., 25(4): 334-342, 2012
 60. A highly coarse-grained model to simulate entangled polymer melts, Zhu, You-Liang; Liu, Hong; Lu, Zhong-Yuan, J. Chem. Phys., 136(14) 文献号: 144903, 2012
 61. Comparison of the FeO₂⁺ and FeS₂⁺ Complexes in the Cyanide and Isocyanide Ligand Environment for Methane Hydroxylation, Tang, Hao; Li, Zhuo; Yang, Yu-Hong; Zhao, Ying; Wan, Su-Qin; Liu, Hui-Ling; Huang, Xu-Ri, J. Comput. Chem., 33(16): 1448-1457, 2012
 62. QM/MM Study on the Catalytic Mechanism of Heme-Containing Aliphatic

- Aldoxime Dehydratase, Pan, Xiao-Liang; Cui, Feng-Chao; Liu, Wei; Liu, Jing-Yao, *J. Phys. Chem. B*, 116(19): 5689-5693, 2012
63. Formaldehyde Decomposition and Coupling on V(100): A First-Principles Study, Wang, Hui; He, Chao-zheng; Huai, Li-yuan; Liu, Jing-yao, *J. Phys. Chem. C*, 116(19): 10639-10648, 2012
 64. Constant pH Molecular Dynamics (CpHMD) and mutation studies: Insights into AaegOBP1 pH-induced ligand releasing mechanism, Chu, Wen-Ting; Wu, Yun-Jian; Zhang, Ji-Long; Zheng, Qing-Chuan; Chen, Lin; Xue, Qiao; Zhang, Hong-Xing, *BBA-Proteins Proteomics*, 1824(7): 913-918, 2012
 65. Mechanism for the formation of benzene in the Titan's atmosphere: A theoretical study on the mechanism of C₄H₂⁺⁺C₂H₄ reaction, Yang, Yuhong; Li, Zhuo; Zhao, Ying; Wan, Suqin; Liu, Huiling; Huang, Xuri; Sun, Chiachung, *Comput. Theor. Chem.*, 991): 66-73, 2012
 66. Homology Modeling And Substrate Binding Study Of Human Kynurenine Aminotransferase III, Xu, Yu; Zheng, Qing-Chuan; Zhang, Hong-Xing; Sun, Chia-Chung, *J. Theor. Comput. Chem.*, 11(4): 855-870, 2012
 67. Molecular dynamics simulation study of the vanillate transport channel of Opdk, Wang, Yibo; Zhao, Xi; Sun, Baili; Yu, Hui; Huang, Xuri, *Arch. Biochem. Biophys.*, 524(2): 132-139, 2012
 68. TDDFT investigation of fluorescence properties of luciferin and oxyluciferin analogs bearing an amino group, Li, Zuo-Sheng; Min, Chun-Gang; Ren, Ai-Min; Zou, Lu-Yi; Xu, Zhong, *J. Photochem. Photobiol. A-Chem.*, 243): 7-16, 2012
 69. Theoretical study of the COLin complexes: Interaction between carbon monoxide and lithium clusters of different sizes, Xi, Yong-Jie; Li, Ying; Wu, Di; Li, Zhi-Ru, *Comput. Theor. Chem.*, 994): 6-13, 2012
 70. Influence of Hyperthermophilic Protein Cren7 on the Stability and Conformation of DNA: Insights from Molecular Dynamics Simulation and Free Energy Analysis, Chen, Lin; Zhang, Ji-Long; Yu, Li-Ying; Zheng, Qing-Chuan; Chu, Wen-Ting; Xue, Qiao; Zhang, Hong-Xing; Sun, Chia-Chung, *J. Phys. Chem. B*, 116(41): 12415-12425, 2012
 71. Stabilities And Fragmentation Behaviors Of Ag-n Clusters (n=2-34), Zhang, Wei; Yan, Shu-Yao; Zhao, Zeng-Xia; Zhang, Hong-Xing, *J. Theor. Comput. Chem.*, 11(5): 953-964, 2012
 72. Mechanism of Ammonia Decomposition and Oxidation on Ir(100): A First-Principles Study, He, Chao-zheng; Wang, Hui; Huai, Li-yuan; Liu, Jing-yao, *J. Phys. Chem. C*, 116(45): 24035-24045, 2012
 73. Successive hydrogenation starting from the edge(s): an effective approach to fine-tune the electronic and magnetic behaviors of SiC nanoribbons, Guan, Jia; Chen, Wei; Zhao, Xiaojie; Yu, Guangtao; Huang, Xuri; Sun, Chiachung, *J. Mater. Chem.*, 22(45): 24166-24172, 2012
 74. Metal hydrides as sodium bond acceptors: hydride-sodium bond in the XH center dot center dot center dot NaH (X = HBe, LiBe, NaBe, HMg, LiMg, and NaMg) complexes, Wang, Shu-Jian; Li, Ying; Wu, Di; Li, Zhi-Ru, *Mol. Phys.*, 110(24): 3053-3060, 2012

75. Effect of dihydropyrazine on structures and charge transport properties of N-heteropentacenes matters: A theoretical investigation, Chen, Xian-Kai; Zou, Lu-Yi; Fan, Jian-Xun; Zhang, Shou-Feng; Ren, Ai-Min, *Org. Electron.*, 13(12): 2832-2842, 2012
76. Theoretical study of nitrogen-rich CN_3^- anion and related salts $\text{M}^+[\text{CN}_3]^-$ ($\text{M} = \text{Li, Na, K}$), Gao, Si-meng; Ding, Yi-hong, *RSC Adv.*, 2(31): 11764-11776, 2012
77. Ab initio Investigation on Unhydrated Ion-associated Species Between Na^+ , Li^+ , Me^+ and SO_4^{2-} Ions, Wan Su-Qin; Zhang Yi; Zhang Hao; Sun Chia-Chung, *Chem. J. Chin. Univ.-Chin.*, 33(7): 1505-1510, 2012
78. Structures and Stabilities of Ni-n ($n=31-35$) Clusters, Song Wei; Lu Wen-cai; Zang Qing-jun; Li Qiu-xia, *Chem. Res. Chin. Univ.*, 28(2): 291-294, 2012
79. Preparation of Nanoporous Carbon Using an Aluminophosphate Framework Template, Zhang Min; Zhu Wanchun; Liu Gang; Zhang Xiuyan; Zu Yanhong; Zhang Wenxiang; Yan Wenfu; Jia Mingjun, *Chin. J. Catal.*, 33(3): 465-472, 2012
80. Does the molecular structure of CaH_2 affect the dihydrogen bonding in CaH_2 center dot center dot center dot HY ($\text{Y} = \text{CH}_3, \text{C}_2\text{H}_3, \text{C}_2\text{H}, \text{CN}, \text{and NC}$) complexes? A quantum chemistry study using MP2 and B3LYP methods, Feng Lu; Bai FuQuan; Wu Yang; Zhang HongXing, *Sci. China-Chem.*, 55(2): 262-269, 2012
81. Surface photovoltage phase spectroscopy study of the photo-induced charge carrier properties of TiO_2 nanotube arrays, Chen LiPing; Xie TengFeng; Wang DeJun; Fan ZhiYong; Jiang TengFei, *Sci. China-Chem.*, 55(2): 229-234, 2012
82. Structural, Electronic and Optical Properties of Multifunctional Iridium(III) and Platinum(II) Metallophosphors for Organic Light-Emitting Diodes, Ran Xueqin; Feng Jikang; Wong Waiyeung; Ren Aimin; Zhou Guijiang; Sun Chiachung, *Chin. J. Chem.*, 30(10): 2431-2439, 2012
83. Theoretical Studies on the Reaction Mechanism of the Cyclization and Dehydrogenation of Open Metallocene, Liu Nan-Nan; Ding Yi-Hong, *Chem. J. Chin. Univ.-Chin.*, 33(10): 2303-2307, 2012
84. Properties and Weak Directionality of the π -Lithium Bond in $\text{C}_2\text{H}_4\text{-nFn}$ center dot center dot center dot LiH ($n=0, 1, 2$) Dimers, Wang Shu-Jian; Li Ying; Wu Di, *Acta Phys.-Chim. Sin.*, 28(12): 2817-2823, 2012
85. Mechanistic study and kinetic properties of the $\text{CF}_3\text{CHO} + \text{Cl}$ reaction, Gao Hong; Wang Ying; Wang Qin; Liu JingYao, *Sci. China-Chem.*, 55(10): 2197-2201, 2012
86. Theoretical Studies on the Basicity of the Boron-substituted Zeolite Interacted by NH_3 , Liu Nan-Nan; Ding Yi-Hong, *Chem. J. Chin. Univ.-Chin.*, 33(9): 2043-2046, 2012
87. Ab initio Investigation on Unhydrated Ion-associated Species Between Na^+ , Li^+ , Mg_2^+ Ions and ClO_4^- , NO_3^- , Wan Su-Qin; Zhang Yi; Zhang Hao; Sun Chia-Chung, *Chem. J. Chin. Univ.-Chin.*, 33(8): 1765-1770, 2012
88. Theoretical Studies on Structural and Spectroscopic Properties of Photoelectrochemical Cell Ruthenium Sensitizers-the Derivatives of N_3 , Chen Jie; Wang Jian; Bai Fu-quan; Zheng Qing-chuan; Zhang Hong-xing, *Chem. Res. Chin.*

- Univ., 28(4): 696-702, 2012
89. A Theoretical Study on Activation of C-H and C-Cl Bonds in CH₃X (X=H, Cl) by Fe²⁺, Sun Xiaoli; Li Jilai; Huang Xuri; Sun Chiachung, *Acta Chim. Sin.*, 70(11): 1245-1249, 2012
 90. Theoretical Study on GSH Activation Mechanism of a New Type of Glutathione Transferase Gtt2, Li Xue; Wu Yun-jian; Li Zhuo; Chu Wen-ting; Zhang Hong-xing; Zheng Qing-chuan, *Chem. Res. Chin. Univ.*, 28(3): 500-502, 2012
 91. Molecular Dynamics of an Extremely Thermophilic Ribose Binding Protein, Feng Xianli; Zhao Xi; Yu Hui; Wang Yibo; Sun Tiedong; Huang Xuri, *Acta Chim. Sin.*, 70(5): 606-610, 2012
 92. Structures and Nonlinear Optical Properties of the Alkalides M(+)-aza222M'(-) (M, M'=Li, Na, K), Fan Li-Tao; Li Ying; Wu Di; Li Zhi-Ru; Sun Chia-Chung, *Acta Phys.-Chim. Sin.*, 28(3): 555-560, 2012
 93. Theoretical Study of CH₃CH=CH₂+O(D-1) Reaction: Mechanism and Kinetics, Wu Nan-nan; Liu Hong-xia; Duan Xue-mei; Liu Jing-yao, *Chem. Res. Chin. Univ.*, 28(1): 147-152, 2012
 94. Molecular Docking of 3-Methylindole-containing Drugs Binding into CYP3A4, Meng Xuan-yu; Li Zhuo; Niu Rui-juan; Zhang Hong-xing; Zheng Qing-chuan, *Chem. Res. Chin. Univ.*, 28(1): 137-141, 2012
 95. Study on Trifluoroacetic Acid Adsorbed on TiO₂ Surface with Density Functional Theory, Cui Wenying; Liu Zizhong; Jiang Yajun; Wang Na; Feng Jikang, *Acta Chim. Sin.*, 70(19): 2049-2058, 2012
 96. Theoretical Investigation on the First Hyperpolarizabilities of M+@H(6)Aza222M'(-)center dot 2MeNH(2)(M, M'=Li, Na, K) Alkalides, Fan Li-Tao; Li Ying; Wu Di; Li Zhi-Ru; Sun Chia-Chung, *Chem. J. Chin. Univ.-Chin.*, 33(10): 2320-2325, 2012