

1. Adsorption and growth morphology of rare-earth metals on graphene studied by ab initio calculations and scanning tunneling microscopy, Xiaojie Liu, C. Z. Wang, M. Hupalo, Y. X. Yao, M. C. Tringides, W. C. Lu, and K. M. Ho, *Phys. Rev. B*, 82, 245408, 2010
2. The effect of viscosity on the phase separation dynamics of binary immiscible mixture coupled with reversible reaction, Hui Li, Hong Liu, Zhong-Yuan Lu\*, Qin Wang, Chia-Chung Sun, *Int. J. Mod. Phys. C*, 21(12), 1479-1488, 2010
3. Releasing of the chromophore from the drug delivery protein C-1027: A molecular dynamics simulations study, Yi-bo Wang, Xi Zhao, Hui Yu, Xu-ri Huang, *J. Struct. Biol.*, 172 (3): 284-293, 2010
4. Structures of Pb-n (n=21-30) clusters from first-principles calculations, Xiao-Ping Li, Wen-Cai Lu, C.Z. Wang, K. M. Ho, *J. Phys.-Condes. Matter*, 22 (46): Art. No. 465501, 2010
5. Theoretical Investigation of the Interaction between Carbon Monoxide and Carbon Nanotubes with Single-Vacancy Defects, Bo Xiao, Jing-xiang Zhao, Yi-hong Ding, Chia-chung Sun, *ChemPhysChem*, 11(16):3505-3510, 2010
6. How Does a Double-Cage Single Molecule Confine an Excess Electron? Unusual Intercage Excess Electron Transfer Transition, Yin-Feng Wang, Zhi-Ru Li, Di Wu, Ying Li, Chia-Chung Sun, Feng Long Gu, *J. Phys. Chem. A*, 114 (43): 11782-11787, 2010
7. Electronic structures and spectroscopic properties of promising highly efficient red phosphorescent Os(II)(LR)(2)(PH3)(2) complexes: a theoretical exploration, Jian-Po Zhang, Bao-Hui Xia, Li Jin, Hong-Xing Zhang, *Theor. Chem. Acc.*, 127 (5-6): 467-474, 2010
8. Perfluorinated exohedral potassium-metallofullerene K center dot center dot center dot C<sub>n</sub>F<sub>n</sub> (n = 20 or 60): partial interior and surface excess electron state, Yin-Feng Wang, Ying Li, Zhi-Ru Li, Fang Ma, Di Wu, Chia-Chung Sun, *Theor. Chem. Acc.*, 127 (5-6): 641-650, 2010
9. Electronic isomerization in fullerene: A density functional trial, X.-Z. Meng, S. Zhang, L.-L. Yu, X.-Q. Ran, W. Q. Tian, *Theochem-J. Mol. Struct.*, 958 (1-3): 122-132, 2010
10. Density Functional Study on the Effect of Substituent Group for the Monomer of Donor-Acceptor Copolymer, Lei Sun, Fu-Quan Bai, Zeng-Xia Zhao, Bao-Zhu Yang, Hong-Xing Zhang, *J. Polym. Sci. Pt. B-Polym. Phys.*, 48 (20): 2099-2107, 2010
11. Theoretical studies of chemisorption of NO<sub>2</sub> molecules on SiC nanotube, Bo Xiao, Jing-xiang Zhao, Yi-hong Ding, Chia-chung Sun, *Surf. Sci.*, 604(21-22):1882-1888, 2010
12. Theoretical studies on the low-lying electronic states of the diazomethyl (HCNN) radical and its ions, Yue-Jie Liu, Zeng-Xia Zhao, Fu-Quan Bai, Ming-Xing Song, Hong-Xing Zhang\*, Chia-Chung Sun, *Theochem-J. Mol. Struct.*, 955 (1-3): 145-151, 2010

13. An "adiabatic-hindered-rotor" treatment allows para-H-2 to be treated as if it were spherical, Hui Li, Pierre-Nicholas Roy, Robert J. Le Roy, *J. Chem. Phys.*, 133 (10): Art. No. 104305, 2010
14. Reaction Mechanism of CH + C<sub>3</sub>H<sub>6</sub>: A Theoretical Study, Yan Li, Hui-ling Liu, Zhong-Jun Zhou, Xu-ri Huang, Chia-chung Sun, *J. Phys. Chem. A*, 114 (35): 9496-9506, 2010
15. Dipole-bound states of the alkali-superhalogen anions: LiBeX<sub>3</sub><sup>-</sup> (X = F, Cl, Br), Jing Tong, Ying Li, Di Wu, Song-Hua Cui, Zhi-Ru Li, Xu-Ri Huang, *Chem. Phys. Lett.*, 496 (1-3): 20-24, 2010
16. Reaction mechanism of CHCl<sup>-</sup> + CSO: A theoretical study, Yan Li, Hui-ling Liu, Zhong-jun Zhou, Yan-bo Sun, Zhuo Li, Xu-ri Huang, Chia-chung Sun, *Theochem-J. Mol. Struct.*, 953 (1-3): 114-122, 2010
17. 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?, Yin-Feng Wang, Wei Chen, Guang-Tao Yu, Zhi-Ru Li, Chia-Chung Sun, *Int. J. Quantum Chem.*, 110 (10): 1953-1963, 2010
18. Theoretical Studies on the Electronic Structures and Spectroscopic Properties of a Series of Novel N-C-N-Coordinating Pt(II) Complexes, Bao-Zhu Yang, Xin Zhou, Tao Liu, Fu-Quan Bai, Hong-Xing Zhang, *Int. J. Quantum Chem.*, 110 (9): 1605-1614, 2010
19. Fluorene-based Oligomers as Red Light-emitting Materials: A Density Functional Theory Study, Xue-Feng Ren, Ai-Min Ren\*, Lu-Yi Zou, Ji-Kang Feng, *Theor. Chem. Acc.*, 126 (5-6): 305-314, 2010
20. Theoretical design study on photophysical property of the B-N derivatives for OLED applications, Lu-Yi Zou, Zi-Long Zhang, Ai-Min Ren\*, Xue-Qin Ran, and Ji-Kang Feng, *Theor. Chem. Acc.*, 126 (5-6): 361-369, 2010
21. Properties of halogen bonds in FArCCX center dot center dot center dot HMY (X = Cl and Br; M = Be and Mg; Y = H, F, and CH<sub>3</sub>) complexes: An ab initio and topological analysis, Shuai Wang, *Theochem-J. Mol. Struct.*, 952 (1-3): 115-119, 2010
22. Toward a full structural characterization of G-quadruplex DNA in aqueous solution: Molecular dynamics simulations of four G-quadruplex molecules, Ming-Hui Li, Quan Luo, Xiang-Gui Xue, Ze-Sheng Li, *Theochem-J. Mol. Struct.*, 952 (1-3): 96-102, 2010
23. Catalytic Mechanism of Hydroxynitrile Lyase from *Hevea brasiliensis*: A Theoretical Investigation, Feng-Chao Cui, Xiao-Liang Pan, Jing-Yao Liu, *J. Phys. Chem. B*, 114 (29): 9622-9628, 2010
24. Efficient porous carbon supported MgO catalysts for the transesterification of dimethyl carbonate with diethyl carbonate, Guoming Zhao, Jinghui Shi, Gang Liu\*, Yan Liu, Zhenlu Wang, Wenxiang Zhang, Mingjun Jia, *Journal of Molecular Catalysis A*, 327(1-2): 32-37, 2010
25. Theoretical Investigation on the Origin of Yellow-Green Firefly Bioluminescence by Time-Dependent Density Functional Theory, Chun-Gang Min, Ai-Min Ren\*,

- Jing-Fu Guo, Lu-Yi Zou, John D. Goddard, Chia-Chung Sun, *ChemPhysChem*, 11 (10): 2199-2204, 2010
26. CASSCF/CASPT2 Calculation of the Low-Lying Electronic States of the CH<sub>3</sub>Se Neutral Radical and Its Cation, Ming-Xing Song, Zeng-Xia Zhao, Fu-Quan Bai, Yue-Jie Liu, Hong-Xing Zhang\*, Chia-Chung Sun, *J. Phys. Chem. A*, 114 (26): 7173-7178, 2010
  27. CaO supported on porous carbon as highly efficient heterogeneous catalysts for transesterification of triacetin with methanol, Yanhong Zu, Gang Liu\*, Zhenlv Wang, Jinghui Shi, Min Zhang, Wenxiang Zhang, Mingjun Jia\*, *Energy & Fuels*, 24, 3810-3816, 2010
  28. Theoretical study of noncovalent functionalization of BN nanotubes by various aromatic molecules, Jing-xiang Zhao, Yi-hong Ding, *Diam. Relat. Mat.*, 19 (7-9): 1073-1077, 2010
  29. 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, Fang Ma, Zhi-Ru Li, Zhong-Jun Zhou, Di Wu, Ying Li, Yin-Feng Wang, Ze-Sheng Li, *J. Phys. Chem. C*, 114 (25): 11242-11247, 2010
  30. Understanding the Borane Analogy in Al<sub>n</sub>H<sub>n+4</sub> (n=5-19): Unprecedented Stability of a Non-Wade-Mingos Cluster Al<sub>8</sub>H<sub>12</sub> Fused by Two T-d-like Al<sub>4</sub>H<sub>6</sub>, Li-juan Fu, Jin Lin, Chang-bin Shao, Yi-hong Ding, *Inorg. Chem.*, 49 (11): 5276-5284, 2010
  31. Geometric structures of Ge-n (n=34-39) clusters, Wei Qin, Wen-Cai Lu, Qing-Jun Zang, Li-Zhen Zhao, Guang-Ju Chen, C. Z. Wang, K. M. Ho, *J. Chem. Phys.*, 132 (21): Art. No. 214509, 2010
  32. Density functional theory study on photophysical properties of the porphyrins derivatives with through-bond energy transfer characters, Xue-Feng Ren, Ai-Min Ren\*, Ji-Kang Feng, Xin Zhou, *Org. Electron.*, 11 (6): 979-989, 2010
  33. Theoretical studies on the adsorption of small molecules on Pt-doped BN nanotubes, Qi Dong, Xi Mao Li, Wei Quan Tian, Xu-Ri Huang, Chia-Chung Sun, *Theochem-J. Mol. Struct.*, 948 (1-3): 83-92, 2010
  34. Theoretical study on the mechanism of the NCO + CH<sub>3</sub> reaction, Ying Zhao, Yan Li, Hui-ling Liu, Xu-ri Huang, Chia-chung Sun, *Theochem-J. Mol. Struct.*, 947 (1-3): 32-39, 2010
  35. Lithium Bonding Interaction Hyperpolarizabilities of Various Li-Bond Dimers, Jing Tong, Ying Li, Di Wu, Zhi-Ru Li, Xu-Ri Huang, *J. Phys. Chem. A*, 114 (18): 5888-5893, 2010
  36. Molecular Dynamics Study on the Interactions of Porphyrin with Two Antiparallel Human Telomeric Quadruplexes, Ming-Hui Li, Quan Luo, Ze-Sheng Li, *J. Phys. Chem. B*, 114 (18): 6216-6224, 2010
  37. Theoretical Study on the Influence of Ancillary Ligand on the Spectroscopic Properties and Electronic Structures of Phosphorescent Pt(II) Complexes, Min Zhang, Yan Li, Ze-Sheng Li, Jia-Zhong Sun, *Int. J. Quantum Chem.*, 110 (6): 1142-1151, 2010

38. A theoretical study on the adsorption of an all-metal aromatic molecule  $\text{Na}_2\text{Al}_4$  on MCM-22 zeolite, Ning He, Hong-Bin Xie, Yi-Hong Ding, *Microporous Mesoporous Mat.*, 130 (1-3): 67-75, 2010
39. A Theoretical Study of the Low-Lying Electronic States of the AICCH Radical and Its Ions, Yue-Jie Liu, Zeng-Xia Zhao, Ming-Xing Song, Hong-Xing Zhang\*, Chia-Chung Sun, *J. Phys. Chem. A*, 114 (15): 5035-5040, 2010
40. Theoretical Study of the Relationships between Excited State Geometry Changes and Emission Energies of Oxyluciferin, Zhong-wei Li, Chun-gang Min, Ai-Min Ren\*, Jing-fu Guo, John D Goddard, Ji-Kang Feng, Liang Zuo, *Bull. Korean Chem. Soc.*, 31 (4): 895-900, 2010
41. Theoretical study for ozonolysis of 1,3-butadiene, Yan Li, Hui-ling Liu, Xu-ri Huang, Zhuo Li, Yan-bo Sun, Chia-chung Sun, *Theochem-J. Mol. Struct.*, 945 (1-3): 120-128, 2010
42. The 3D structures of G-Quadruplexes of HIV-1 integrase inhibitors: molecular dynamics simulations in aqueous solution and in the gas phase, Ming-Hui Li, Yi-Han Zhou, Quan Luo, Ze-Sheng Li, *J. Mol. Model.*, 16 (4): 645-657, 2010
43. Reaction of Cl with  $\text{CF}_3\text{CH}_2\text{OCHO}$ : A mechanistic and kinetic study, Hong-xia Liu, Yu-chang Liu, Su-qin Wan, Jing-yao Liu, *Theochem-J. Mol. Struct.*, 944 (1-3): 124-131, 2010
44. Lithium salt of end-substituted nanotube: Structure and large nonlinear optical property, Fang Ma, Zhong-Jun Zhou, Zhi-Ru Li, Di Wu, Ying Li, Ze-Sheng Li, *Chem. Phys. Lett.*, 488 (4-6): 182-186, 2010
45. Theoretical Mechanistic Study on the Ion-Molecule Reaction of  $\text{CHCl}_2$  with  $\text{CS}_2$ , Yan Li, Hui-ling Liu, Yan-bo Sun, Zhuo Li, Xu-ri Huang, Chia-chung Sun, *J. Phys. Chem. A*, 114 (8): 2874-2884, 2010
46. A Simulation Model for the Hierarchical Self-Assembly of Soft Disklike Micelles, Zhan-Wei Li, Zhao-Yan Sun, Zhong-Yuan Lu, *J. Phys. Chem. B*, 114, 2353-2358, 2010
47. Theoretical study on photophysical properties of angular-shaped mercury(II) bis(acetylide) complexes as light-emitting materials, Xue-Qin Ran, Ji-Kang Feng\*, Wai-Yeung Wong\*, Ai-Min Ren, Suk-Yue Poon, Chia-Chung Sun, *Chem. Phys.*, 368 (1-2): 66-75, 2010
48. Comparative Study on the Catalytic Properties of Amino-Functionalized Silica Materials for the Transesterification of Dimethyl Oxalate with Phenol, G. Liu, Y. Liu, X.Y. Zhang, X.L. Yuan, M. Zhang, W.X. Zhang, M.J. Ji a, *Journal of Colloid and Interface Science*, 342, 467-473, 2010
49. Electronic and Charge-transport Properties of 1,1,2,3,4,5-hexaphenylsilole (HPS) crystal from Theoretical Calculations, Yu-Hua Liu, Yu Xie, Zhong-Yuan Lu, *Chem. Phys.*, 367(2-3), 160-166, 2010
50. Direct Ab Initio Dynamics Studies On The Reaction Of Methanethiol With Chlorine Atoms, Yong-Xia Wang, Xue-Mei Duan, Qin Wang, Li Wang, Jing-Yao Liu, Chia-Chung Sun, *J. Theor. Comput. Chem.*, 9 (1): 265-277, 2010
51. DFT/TD-DFT Investigation on Ir(III) Complexes with N-Heterocyclic Carbene Ligands: Geometries, Electronic Structures, Absorption, and Phosphorescence

- Properties, Tao Liu, Bao-Hui Xia, Qing-Chuan Zheng, Xin Zhou, Qing-Jiang Pan, Hong-Xing Zhang, *J. Comput. Chem.*, 31 (3): 628-638, 2010
52. 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), Y.-H. Cui, W. Q. Tian\*, J.-K. Feng, and D.-L. Chen, *J. Nanopart. Res.*, 12 (2): 429-438, 2010
  53. Theoretical study of one- and two-photon absorption properties of expanded donor-acceptor calix[4]arenes, Wen-Chao Li, Ji-Kang Feng\*, Ai-Min Ren, Xiang-Biao Zhang, Chia-Chung Sun, *J. Phys. Org. Chem.*, 23 (2): 126-133, 2010
  54. Layered structure in compatible binary polymer brushes with high graft density, Yao-Hong Xue, Hong Liu, Zhong-Yuan Lu\*, Xue-Zhang Liang, *J. Chem. Phys.*, 132(4), 044903, 2010
  55. A Time-Dependent Density Functional Theory Investigation on the Origin of Red Chemiluminescence, Chun-Gang Min, Ai-Min Ren\*, Jing-Fu Guo, Zhong-Wei Li, Lu-Yi Zou, John D. Goddard, Ji-Kang Feng, *ChemPhysChem*, 11 (1): 251-259, 2010
  56. Excess Electron is Trapped in a Large Single Molecular Cage C60F60, Yin-Feng Wang, Zhi-Ru Li, Di Wu, Chia-Chung Sun, Feng-Long Gu, *J. Comput. Chem.*, 31 (1): 195-203, 2010
  57. Unbinding of glucose from human pulmonary surfactant protein D studied by steered molecular dynamics simulations, Ji-Long Zhang, Qing-Chuan Zheng, Hong-Xing Zhang, *Chem. Phys. Lett.*, 484 (4-6): 338-343, 2010
  58. Comparative study on catalytic properties over different amino-functionalized silica materials for the transesterification of dimethyl oxalate with phenol, Yan Liu, Guoming Zhao, Wanchun Zhu, Jing Wang, Gang Liu, Wenxiang Zhang, Mingjun Jia\*, *Journal of the Brazilian Chemical Society*, 21(12), 2254-2261, 2010
  59. Molecular dynamics simulations investigation of neocarzinostatin chromophore-releasing pathways from the holo-NCS protein, Xi Zhao, Song Wang, Xue-feng Gao, Xu-ri Huang, Chia-chung Sun, *J. Struct. Biol.*, 169 (1): 14-24, 2010
  60. CASPT2 and CASSCF studies on the low-lying electronic states of the HCCO radical and its anion, Yue-Jie Liu, Zeng-Xia Zhao, Hong-Xing Zhang\*, Chia-Chung Sun, *Theor. Chem. Acc.*, 125 (1-2): 65-73, 2010
  61. Push-pull electron effects of the complexant in a Li atom doped molecule with electride character: a new strategy to enhance the first hyperpolarizability, Zhen-Bo Liu, Zhong-Jun Zhou, Ying Li, Zhi-Ru Li, Rong Wang, Qing-Zhong Li, Yang Li, Feng-Yan Jia, Yin-Feng Wang, Zong-Jun Li, Jian-Bo Cheng, Chia-Chung Sun, *Phys. Chem. Chem. Phys.*, 12 (35): 10562-10568, 2010
  62. Zinc (0) chemistry: does the missing 18-electron zinc tricarbonyl really exist?, Lin Jin, Li-Juan Fu, Yi-Hong Ding, *Phys. Chem. Chem. Phys.*, 12 (36): 10956-10962, 2010
  63. Is the planar hexacoordinate nitrogen molecule NB6- viable?, Chang-Bing Shao, Yi-Hong Ding, *Phys. Chem. Chem. Phys.*, 12 (40): 13153-13157, 2010

64. Pentaatomic planar tetracoordinate carbon molecules [XCA13](q) [(X,q) = (B,-2), (C,-1), (N,0)] with C-X multiple bonding, Zhong-Hua Cui, Chang-Bing Shao, Si-Meng Gao, Yi-Hong Ding, *Phys. Chem. Chem. Phys.*, 12 (41): 13637-13645, 2010
65. Mobius basket molecule: structure and properties, Yin-Feng Wang, Zhuo Li, Ying Li, Zhi-Ru Li, Zong-Jun Li, Di Wu, Fang Ma, Chia-Chung Sun, *Phys. Chem. Chem. Phys.*, 12 (31): 8847-8855, 2010
66. Potential energy surface survey of Al<sub>3</sub>H<sub>7</sub>: borane analogue or not?, Li-Juan Fu, Chang-Bin Shao, Lin Jin, Yi-Hong Ding, *Mol. Phys.*, 108 (13): 1715-1722, 2010
67. Effect of substitution and cooperativity on the Cl-F blue shift in single-electron halogen-bonded H<sub>3</sub>C center dot center dot center dot ClF complex, Zhong-Jun Zhou, Hui-Ling Liu, Xu-Ri Huang, Qing-Zhong Li, Chia-Chung Sun, *Mol. Phys.*, 108 (15): 2021-2026, 2010
68. Optical and Electronic Properties of Doubly Ortho-linked cis-4,4'-Bis(diarylamino)stilbene/Fluorene Hybrids, Yan-Ling Liu, Xue-Qin Ran, Ji-Kang Feng\*, Ai-Min Ren, Lu-Yi Zou, *Aust. J. Chem.*, 63 (1): 125-130, 2010
69. Insight into the Dynamic Interaction of Different Carbohydrates with Human Surfactant Protein D: Molecular Dynamics Simulations, Ji-Long Zhang, Qing-Chuan Zheng, Hong-Xing Zhang, *J. Phys. Chem. B*, 114 (21): 7383-7390, 2010
70. Influence of Activation/Deactivation Process on the Dynamics of Surface Initiated Polymerization with High Grafting Density, Liu Yu-Hua; Li Min; Liu Hong; Lue Zhong-Yuan; Zhang Zuo-Guang, *Chem. J. Chin. Univ.-Chin.*, 31(12):2458-2462, 2010
71. Effects of electric field on the structures and electronic properties of N@C<sub>60</sub>, P@C<sub>60</sub>, and As@C<sub>60</sub>, Q. Dong, W.Q. Tian\*, W.Q. Li\*, X.-D. Sun, C. C. Sun, *Chem. J. Chin. Univ.-Chin.*, 31: 2254-2259, 2010
72. Fragmentation Behavior and Ionization Potentials of Lead Clusters Pb-n (n ≤ 30), Li Xiao-ping; Zhang Wei; Lue Wen-cai; Wang Cai-zhuang; Ho Kai-ming, *Chem. Res. Chin. Univ.*, 26 (6): 996-1001, 2010
73. Theoretical Studies on Reaction Mechanism of CH<sub>4</sub> and N<sub>2</sub>(+) Reaction, Wang Lei, Liu Hui-Ling, Yang Guang-Hui, Huang Xu-Ri, *Chem. J. Chin. Univ.-Chin.*, 31 (10): 2015-2018, 2010
74. Photodissociation Mechanism of Cyanogen Azide, Ci Cheng-Gang; Duan Xue-Mei; Liu Jing-Yao; Sun Chia-Chung, *Acta Phys.-Chim. Sin.*, 26 (10): 2787-2792, 2010
75. Theoretical Investigation of the Key Reaction for the Chemiluminescence of Cypridina Luciferin Analogues, Ying Sun, Ai-Min Ren\*, Chun-Gang Min, Lu-Yi Zou, Xue-Feng Ren, *Acta Phys.-Chim. Sin.*, 26 (10): 2779-2786, 2010
76. Insight into Reaction Mechanism of Sirtuins via Molecular Simulation and Density Functional Theory Study, Yong-Shan Zhao, Rui-Zhe Hou, Hong-Xing Zhang, Qing-Chuan Zheng\*, Chia-Chung Sun, *Chem. Res. Chin. Univ.*, 26 (5): 833-837, 2010

77. The Influence of Solvent Size on the Structural Properties of Bottle-Brush Polymers, Ying-Tao Liu, Hong Liu, Yu-Hua Liu, Zhong-Yuan Lu, Chem. Res. Chin. Univ., 26(5), 838-841, 2010
78. Theoretical Studies on the Low-Lying Excited States of Aluminum Cyanide (AICN) and Its Ions, Yue-Jie Liu, Zeng-Xia Zhao, Ming-Xing Song, Hong-Xing Zhang\*, Chia-Chung Sun, Acta Chim. Sin., 68 (17): 1687-1691, 2010
79. Ab-initio Investigation on Ion-associated Species and Association Process in NaClO<sub>4</sub> Solution, Zhang Hao; Yu Jian-Kang; Sun Chia-Chung, Chem. J. Chin. Univ.-Chin., 31 (8): 1600-1604, 2010
80. Ab-initio Investigation on the Ion-associated Species and Process in Mg(ClO<sub>4</sub>)<sub>2</sub> Solution, Zhang Hao; Yu Jiankang; Sun Chiachung, Acta Chim. Sin., 68 (14): 1363-1369, 2010
81. Theoretical Study on the Mechanism and Dynamic of CF<sub>3</sub> CH<sub>2</sub> CH<sub>3</sub> Reaction with OH Radicals, Wang Yong-Xia; Gao Hong; Wang Qin; Liu Jing-Yao, Chem. J. Chin. Univ.-Chin., 31 (6): 1240-1245, 2010
82. Theoretical Studies on the Structures and Stabilities of [MA<sub>15</sub>]<sup>(+)</sup> (M = Si, Ge, Sn, Pb), He Hai-Peng, Cui Zhong-Hua, Ding Yi-Hong, Chem. J. Chin. Univ.-Chin., 31 (4): 772-776, 2010
83. Fragmentation Behavior and Ionization Potentials of Aluminum Clusters Al<sub>n</sub> (n ≤ 40), Wei Zhang, Zhuo Li, Gang Zhang, and Wen-Cai Lu, Chem. Res. Chin. Univ., 26 (2): 294-299, 2010
84. Theoretical Study on Structures and UV-Vis Spectra of Macrocyclic Thiophene Derivatives, 黄双, 任爱民, 李卓, 赵杨, 闵春刚, Chem. J. Chin. Univ.-Chin., 31 (3): 553-558, 2010
85. Homology Modeling of Human Extracellular Signal-regulated Kinase 1 and Docking and Reconstitution of Its Inhibitors, Ji-long Zhang, Rui-zhe Hou, Zhuo Li, Qing-chuan Zheng\*, Hong-xing Zhang, Acta Chim. Sin., 68 (3): 222-226, 2010
86. Theoretical Study on Isomerization Stability of B<sub>4</sub>O Molecule, Shao Chang-Bin, Jin Lin, Ding Yi-hong, Chem. J. Chin. Univ.-Chin., 31 (2): 348-352, 2010
87. Star-shaped Organic Molecules That Comprise a 1,3,5-Trisubstituted Benzene Core and Three Oligoaryleneethynylene Arms as Light-emitting Materials, an-Ling Liu, Ji-Kang Feng\*, Xue-Qin Ran, Ai-Min Ren, Chin. J. Chem., 28 (2): 199-207, 2010
88. Theoretical Studies on the Penta-atomic Planar Coordinate Carbon Molecules [CA<sub>13</sub>X] and [CA<sub>13</sub>X]<sup>(-)</sup> (X=Sn, Pb), He Haipeng, Ding Yihong, Acta Chim. Sin., 68 (1): 13-18, 2010
89. Theoretical Studies for One- and Two-photon Absorption Properties of 3,6- and 2,7-Carbazole Derivatives, Wen-Chao Li, Ji-Kang Feng\*, Ai-Min Ren, Chia-Chung Sun, Xiao-Qiang Yu, Jun-Jie Wang, Chem. J. Chin. Univ.-Chin., 31 (1): 100-105, 2010
90. Preparation of Mesoporous TiO<sub>2</sub>/CdS Thin Film Photoelectrode Through Electrodeposition, Zhou Wei; Fu Hong-Gang; Pan Kai; Tian Chun-Gui; Tian

- Guo-Hui; Ren Zhi-Yu; Qu Yang; Sun Chia-Chung, Chem. J. Chin. Univ.-Chin., 31 (1): 112-116, 2010
91. ab initio Study on the Spectroscopy of H<sub>2</sub>CCC, Xin Shu, Zeng-Xia Zhao, Hong-Xing Zhang\* Chia-Chung Sun, Chem. J. Chin. Univ.-Chin., 31 (1): 125-129, 2010
  92. Structural and Optical Properties of meso-Substituted Porphyrin Derivatives, Xue-Feng Ren, Ai-Min Ren\*, Qin Wang, Ji-Kang Feng, Acta Phys.-Chim. Sin., 26 (1): 110-114, 2010
  93. Electronic Structures and Optical Properties of Indolocarbazole Isomers, Hui-Ping Wang, Fu-Quan Bai, Qing-Chuan Zheng, Zeng-Xia Zhao, Xiao-Jie Zhao, Hong-Xing Zhang, Acta Phys.-Chim. Sin., 26 (1): 115-119, 2010
  94. Direct Ab initio Dynamics on the Reaction of Methanethiol and Hydrogen Atom, Wang Yong-Xia; Duan Xue-Me); Wang Qin; Liu Jing-Yao, Acta Phys.-Chim. Sin., 26 (1): 183-187, 2010
  95. Theoretical Design of Catalytic Domain of Abzyme Se-scFv2F3 by Introducing a Catalytic Triad, Luo Quan; Zhou Yi-han; Yao Yuan; Li Ze-sheng, Chem. Res. Chin. Univ., 26 (1): 118-121, 2010
  96. Theoretical Study on Static First Hyperpolarizabilities of Hypervalent Compounds F<sub>n</sub>Lin+1 (n=1-3), Li Ying; Wu Di, Chem. J. Chin. Univ.-Chin., 31 (9): 1811-1814, 2010