Resume of Wenli Zou

CONTACTS

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EDUCATION

Sep, 94—Jun, 98	Department of Physics, Nankai University, China	BS, Optics
Sep, 98—Jun, 03	Institute of Modern Optics, Nankai University, China	PHD, Optics

RESEARCH EXPERIENCE

May, 2010—Present, Department of Chemistry, Southern Methodist University
Advisor: Prof. Dr. Dieter Cremer
- Method developments

Jun, 2007—Apr, 2010, Dept. of Chem. and Biochem., The University of Texas at Austin
Advisor: Prof. Dr. James E. Boggs
- Intramolecular dynamics (Jahn-Teller Effect)

Jul, 2003—May, 2007, ITCC, College of Chemistry, Peking University, China
Advisor: Prof. Dr. Wenjian Liu
- Development of relativistic LCAO-CO-DFT program based on BDF
- Ab initio study on low-lying electronic states of heavy-element systems

Sep, 1998—Jun, 2003, Institute of Modern Optics, Nankai University, China
Mentor: Prof. Meirong Lin
- Laser induced fluorescence spectra and dynamic characteristics of molecules
- Ab initio study on low-lying electronic states of diatomic molecules

SCIENTIFIC INTERESTS

1. Development of ab initio and/or DFT electronic structure programs.
2. Point group, rod group, layer group, and space group symmetries.
3. Relativistic quantum chemistry of molecules and solids.
4. Instabilities, excited states, and UV-Vis spectra of small molecules.

SKILLS

1. Computer languages: FORTRAN and C.
2. Proficiency with various quantum chemistry programs: ADF, CFOUR, DALTON, DIRAC, GAMESS, GAUSSIAN, MOLCAS, MOLFDIR, MOLPRO, NWCHEM, PC-GAMESS, and so on.
3. Experienced with experimental techniques on laser spectroscopy.

PUBLICATIONS

1. Liu Y, Bersuker IB, Zou WL, et al., Pseudo Jahn-Teller versus Renner-Teller effects in the instability of linear molecules, CHEM. PHYS. 376, 30 (2010).
2. Zou WL, Xu D, Zajac P, et al., Symmetry breaking in linear ZnCl2+: A theoretical study, J. MOL. STRUC. 978, 263 (2010).
3. Zou WL, Liu Y, Boggs JE, Relativistic ab initio study on PtF and HePtF, DALTON TRANS. 39, 2023 (2010).
4. Zhang Y, Xu WH, Sun QM, Zou WL, Liu WJ, Excited States of OsO4: A Comprehensive Time-Dependent Relativistic Density Functional Theory Study, J. COMPUT. CHEM. 31, 532 (2010).
5. Zou WL, Liu Y, Liu WJ, et al., He@Mo6Cl8F6: A Stable Complex of Helium, J. PHYS. CHEM. A, 114, 646 (2010).
6. Zou WL, Liu Y, Boggs JE, Theoretical study of RgMF (Rg = He, Ne; M = Cu, Ag, Au): Bonded structures of helium, CHEM. PHYS. LETT. 482, 207 (2009).
7. Liu Y, Bersuker IB, Zou WL, et al., Combined Jahn-Teller and Pseudo-Jahn-Teller Effect in the CO3 Molecule: A Seven-State Six-Mode Problem, J. CHEM. THEO. COMPUT. 5, 2679 (2009).
8. Liu Y, Zou WL, Bersuker IB, et al., Symmetry breaking in the ground state of BNB: A high level multireference study, J. CHEM. PHYS. 130, 184305 (2009).
9. Zou WL, Boggs JE, Theoretical study of the electronic states of CuCl2, J. CHEM. PHYS. 130, 154313 (2009).
10. Xu WH, Ma JY, Peng DL, Zou WL, Liu WJ, Staemmler V., Excited states of ReO4-: A comprehensive time-dependent relativistic density functional theory study, CHEM. PHYS. 356, 219 (2009).
11. Zou WL, Liu WJ, Comprehensive Ab Initio Calculation and Simulation on the Low-Lying Electronic States of TlX (X = F, Cl, Br, I, and At), J. COMPUT. CHEM. 30, 524 (2009).
12. Zou W, Bersuker IB, Boggs JE, Do non-centro-symmetric linear X-Y-X molecules exist? The case for the (I) (2)Pi(u) state of CuCl2, J. CHEM. PHYS. 129, 114107 (2008).
13. Zou WL, Boggs JE, Theoretical study on low-lying electronic states of NiH2, J. PHYS. CHEM. A 112, 4100 (2008).
14. Zou WL, Liu WJ, Theoretical study on the low-lying electronic states of NiH and NiAt, J. COMPUT. CHEM. 28, 2286 (2007).
15. Zou WL, Liu WJ, Comprehensive theoretical studies on the low-lying electronic states of NiF, NiCl, NiBr, and NiI, J. CHEM. PHYS. 124, 154312 (2006).
16. Peng DL, Zou WL, Liu WJ, Time-dependent quasirelativistic density-functional theory based on the zeroth-order regular approximation, J. CHEM. PHYS. 123, 144101 (2005).
17. Gao J, Zou WL, Liu WJ, et al. Time-dependent four-component relativistic density-functional theory for excitation energies. II. The exchange-correlation kernel, J. CHEM. PHYS. 123, 054102 (2005).
18. Zou WL, Liu WJ, Extensive theoretical studies on the low-lying electronic states of indium monochloride cation, InCl+, J. COMPUT. CHEM. 26, 106 (2005).

19. Yang XZ, Lin MR, Zou WL, et al., Spectroscopic constants of gallium monohalides: a DFT study, THEOCHEM, 668, 209 (2004).
20. Yang XZ, Lin MR, Zou WL, et al., An ab initio study of the ground and valence excited states of GaCl, J. PHYS. B ATOM. MOL. OPT. PHYS. 36, 4651 (2003).
21. Zou WL, Lin MR, Yang XZ, et al., Ab initio calculations on the ground and low-lying excited states of InI, MOL. PHYS. 101, 2963 (2003).
22. Yang XZ, Lin MR, Zou WL, et al., Experimental and theoretical study on the electronic states and spectra of InBr, PHYS. CHEM. CHEM. PHYS. 5, 4786 (2003).
23. Zou WL, Lin MR, Yang XZ, et al., Ab initio calculations on the ground and low-lying excited states of InCl, J. CHEM. PHYS. 119, 3721 (2003).
24. Yang XZ, Lin MR, Zou WL, et al., Time-dependent density functional theory study of the electronic states of BI, J. PHYS. B ATOM. MOL. OPT. PHYS. 36, 2283 (2003).
25. Yang XZ, Lin MR, Zou WL, et al., Ab initio study on the ground and low-lying excited states of GaH, CHEM. PHYS. LETT. 372, 355 (2003).
26. Zou WL, Lin MR, Yang XZ, et al., Ab initio calculations on the ground and low-lying excited states of InH, PHYS. CHEM. CHEM. PHYS. 5, 1106 (2003)
27. Zou WL, Lin MR, Yang XZ, et al., Time-dependent DFT study on the electronic states of BBr, CHEM. PHYS. LETT. 369, 214 (2003).
28. Yang XZ, Lin MR, Zou WL, et al., DFT study on the ground and the first excited states of gallium monohalides, CHEM. PHYS. LETT. 362, 190 (2002).
29. Zou WL, Lin MR, Yang XZ, et al., Theoretical study of C-1 Pi-X-1 Sigma+ transition of InCl, CHEM. PHYS. LETT. 356, 523 (2002).
30. Li YJ, Lin MR, Zou WL, et al., Lifetime measurements of the C-1 Pi(1) and B-3 Pi(1) electronic states of InCl by laser induced fluorescence, MOL. PHYS. 98, 1365 (2000).
31. Li YJ, Lin MR, Zhang BZ, Zhao QC, Zou WL, Chen WJ., Lifetime measurement of the A(3)II(0) electronic state of InCl by laser induced fluorescence, MOL. PHYS. 97, 607 (1999).