Zhijun Zhang

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Education

- **Ph. D.** Institute of Chemistry, Chinese Academy of Sciences 2003-2011
- **B. Sc.** College of Chemistry and Molecular Engineering, Peking University 1999-2003

Research Experience

- Postdoc Peking University Apr. 2015–Present
  Research on molecular vibrational spectroscopy, using the Path Integral Liouville Dynamics method.
- Research Assistant Peking University Dec. 2014–Mar. 2015
  Research on molecular vibrational spectroscopy, using Molecular Dynamics method.
- Thermodynamics calculation engineer Process Integration Limited Aug. 2011–Nov. 2014
  Responsible for the property package used for process integration, including the thermodynamic properties for water and steam, petroleum fractions, crude oil and residues. Implement the methods and algorithms to C++ code.
- Ph. D. research Institute of Chemistry, Chinese Academy of Sciences Sep. 2003–Jul. 2011
  Research on molecular reaction dynamics, involved in three areas as below:
  1. Molecular dynamics simulation of the H+SiH_4 abstraction reaction, using the variational transition state theory.
  2. Quantum dynamics studies of the CH_2 system, including the non-adiabatic effect (Renner-Teller effect).
  3. Full-dimensional quantum mechanical calculations of the vibrational states of acetylene, with the PIST method.

Research Interests

- Theoretical and computational chemistry;
- Quantum dynamics; non adiabatic dynamics; molecular spectroscopy and dynamics;
- Thermodynamic properties of liquids and gases.

Publications

1. Zhijun Zhang, Bin Li, Zhitao Shen, Yinghui Ren, Wensheng Bian (**2012**).
   Efficient quantum calculation of the vibrational states of acetylene.
   Chem. Phys. 400, 1–7.

2. Zhijun Zhang, Haitao Ma and Wensheng Bian (**2011**).
   Accurate quantum mechanical study of the Renner-Teller effect in the singlet CH_2.
   J. Chem. Phys. 135, 154303.

3. Jianwei Cao, Zhijun Zhang, Chunfang Zhang, Wensheng Bian and Yin Guo (**2011**).
   Kinetic study on the H+SiH_4 abstraction reaction using an *ab initio* potential energy surface.
   J. Chem. Phys. 134, 024315.

4. Jianwei Cao, Zhijun Zhang, Chunfang Zhang, Kun Liu, Manhui Wang and Wensheng Bian (**2009**).
   Quasiclassical trajectory study of H+SiH_4 reactions in full-dimensionality reveals atomic-level mechanisms.
   Proc. Natl. Acad. Sci. U.S.A. 106, 13180–13185.

5. Guoying Zuo, Zhijun Zhang, Lirong Chen, Xiaojie Xu (**2005**).
   Chemical Constituents of Tibetan Herbal Medicine *Saxifraga melanocentra*.
   Acta Botanica Yunnanica 27(6): 691–694.

Conference Presentations

1. Poster presentation at 15th International Congress of Quantum Chemistry (satellite meeting at Peking University and main conference at Tsinghua University), Beijing, China June 4–13, 2015
   Study on Path Integral Liouville Dynamics

2. Poster presentation at 5th International Conference on Theoretical Chemistry, Molecular Modeling and Life Sciences (ICTCLS'10), Nandaihe, China August 8–11, 2010
   Quantum dynamical study of Renner-Teller effects on vibrational spectra of singlet CH_2

3. Poster presentation at 11th National Conference on Chemical Kinetics, Yichang–Chongqing, China August 13–17, 2009
   Quantum dynamical study of Renner-Teller effects on vibrational spectra of singlet CH_2

4. Poster presentation at 12th International Symposium of Stereodynamics of Chemical Reactions, Dalian, China October 13–17, 2008
   Quantum dynamical study of Renner-Teller effects on vibrational spectra of singlet CH_2

Programming Skills

- over 50000 lines: C++
- over 10000 lines: Fortran, LaTeX
- Familiar: Shell scripts, Python, html+css

Last updated: July 5, 2015