Curriculum Vitae
Tao Zeng

Education and Research Experience

Title	Period	Institute, Research Focus, and Supervisors
PDF	2013.7 - present	Department of Chemistry and Chemical Biology, Cornell University Theoretical investigations in organic molecule excited state and radical chemistry Prof. Nandini Ananth and Prof. Roald Hoffmann
PDF	2011.1 – 2013.6	Department of Chemistry, University of Waterloo Theoretical investigations in molecular spectroscopy and microscopic superfluidity Prof. Pierre-Nicholas Roy
PhD	2005.9 – 2010.11	Department of Chemistry, University of Alberta Relativistic quantum chemistry and pseudopotential methodology Prof. Mariusz Klobukowski
MSc	2002.9 – 2005.7	Institute of Coal Chemistry, Chinese Academy of Sciences Theoretical investigations in CO adsorption on catalysts during the Fischer-Tropsch process Prof. Haijun Jiao
BSc	1998.9 – 2002.7	Department of Chemistry, Jinan University Undergraduate research: Developing heteropolyacid catalyst for ester synthesis under the supervision of Prof. Yuanming Zhang

Scholarships and Awards

Name	Year	Source of funds/Issuing Organization
Banting Postdoctoral Fellowship	2013 - 2015	NSERC, Canada
John Charles Polanyi Prize	2012	Ontario Council on Graduate Studies
MRI Postdoctoral Fellowship	2011 - 2013	Ontario Ministry of Research and Innovation
NSERC Postdoctoral Fellowship	2011 - 2013	NSERC, Canada
Governor General of Canada's Gold Medal	2011	Office of Governor General of Canada
Ralph Steinhauer Award of Distinction	2010 - 2011	Alberta Scholarship Program
Andrew Stewart Memorial Graduate Prize	2009	University of Alberta
Honorary Izaak Walton Killam Memorial Scholarship	2007 - 2009	Killam Trusts
Alberta Ingenuity Student Scholarship	2006 - 2010	Alberta Ingenuity Funds
Provost Doctoral Entrance Award	2005 - 2006	University of Alberta
Excellent Master Graduate Student of Shanxi Province	2005	Shanxi Province, China
Excellent Student Award of Graduate School of Chinese Academy of Sciences	2003	Graduate School of Chinese Academy of Sciences
Excellent Graduate of Jinan University	2002	Jinan University
1st class Excellent Student	1999 - 2002	Jinan University
2nd class Excellent Student	1998 - 1999	Jinan University

Research Interests

Energy Science; quantum chemistry; path integral simulation; hydrogen storage; organic photovoltaics; excited state chemistry; spin-orbit coupling; Jahn-Teller effect; electronic energy surface hopping; pseudopotential method.

Research Contributions

Peer-Reviewed Papers

Cornell University:

32. **T. Zeng**, H. Wang, Y. Lu, Y. Xie, H. Wang, H. F. Schaefer, N. Ananth, and R. Hoffmann "Tuning spin-states of carbynes and silylynes: a long jump with one leg." *J. Am. Chem. Soc.* **2014**, *136*, 13388-13398.

31. **T. Zeng***, N. Ananth, and R. Hoffmann "Seeking small molecules for singlet fission: a heteroatom substitution strategy." *J. Am. Chem. Soc.* **2014**, *136*, 12638-12647. (* corresponding author)

30. **T. Zeng**, R. Hoffmann, and N. Ananth "The low-lying electronic states of pentacene and their roles in singlet fission." *J. Am. Chem. Soc.* **2014**, *136*, 5755-5764 (JACS Spotlights).

University of Waterloo:

29. Y.-T. Ma, **T. Zeng**, and H. Li "Analytical Morse/long-range model potential and predicted infrared and microwave spectra for a symmetric top-atom dimer: a case study of CH_3F-He." *J. Chem. Phys.* **2014**, *140*, 214309, 13 pages.

28. **T. Zeng** and P.-N. Roy "Microscopic molecular superfluid response: theory and simulations." *Rep. Prog. Phys.* **2014**, *77*, 046601, 40 pages.

27. G. Guillon, **T. Zeng**, and P.-N. Roy "A new post-quantization constrained propagator for rigid tops for use in path integral quantum simulations." *J. Chem. Phys.* **2013**, *139*, 184115, 10 pages.

26. S. Constable, M. Schmidt, C. Ing, **T. Zeng**, and P.-N. Roy "Langevin equation path integral ground state." *J. Phys. Chem. A* **2013**, *117*, 7461-7467.

25. G. Guillon, **T. Zeng**, and P.-N. Roy "On the origin and convergence of a 'Rattle and Shake' propagator for path integral quantum simulations." *J. Chem. Phys.* **2013**, *138*, 184101, 11 pages.

24. Y. Tritzant-Martinez, **T. Zeng**, A. Broom, E. Meiering, R. J. Le Roy, and P.-N. Roy "On the analytical representation of free energy profiles with a Morse/Long-Range model: application to the water dimer." *J. Chem. Phys.* **2013**, *138*, 234103, 12 pages.

23. **T. Zeng**, G. Guillon, and P.-N. Roy "Probing the superfluid response of *para*-hydrogen with a sulfur dioxide dopant." *J. Phys. Chem. Lett.* **2013**, *4*, 2391-2396.

22. **T. Zeng**, H. Li, and P.-N. Roy "Simulating asymmetric top impurities in superfluid clusters: a *para*-water dopant in *para*-hydrogen." *J. Phys. Chem. Lett.* **2013**, *4*, 18-22.

21. C. Ing, J. Yang, K. Hinsen, **T. Zeng**, H. Li, and P.-N. Roy "A path-integral Langevin equation treatment of low-temperature doped helium clusters." *J. Chem. Phys.* **2012**, *136*, 224309, 12 pages.

20. **T. Zeng**, H. Li, R. J. Le Roy, and P.-N. Roy "Adiabatic-hindered-rotor treatment for *para*-H_2 and H_2O system." *J. Chem. Phys.* **2011**, *135*, 094304, 15 pages.

University of Alberta:

19. **T. Zeng**, D. G. Fedorov, M. W. Schmidt, and M. Klobukowski "Natural spinors reveal how the spin-orbit coupling affects the Jahn-Teller distortions in the hexafluorotungstate(V) anion." *J. Chem. Theory Comput.* **2012**, *8*, 3061-3071.

18. H. Mori, **T. Zeng**, and M. Klobukowski "Assessment of chemical core potentials for the computation on enthalpies of formation of transition-metal complexes." *Chem. Phys. Lett.* **2012**, *521*, 150-156.

17. **T. Zeng**, D. G. Fedorov, M. W. Schmidt, and M. Klobukowski "Effects of spin-orbit coupling on covalent bonding and the Jahn-Teller effect are revealed with the natural language of spinors." *J. Chem. Theory Comput.* **2011**, *7*, 2864-2875.

16. **T. Zeng**, D. G. Fedorov, M. W. Schmidt, and M. Klobukowski "Two-component natural spinors from two-step spin-orbit coupled wave functions." *J. Chem. Phys.* **2011**, *134*, 214107, 9 pages.

15. **T. Zeng**, D. G. Fedorov, and M. Klobukowski "Performance of dynamically weighted MCSCF and spin-orbit coupling calculations of diatomic molecules of Group 14 elements." *J. Chem. Phys.* **2011**, *134*, 024108, 11 pages.

14. **T. Zeng**, D. G. Fedorov, and M. Klobukowski "Model core potentials of p-block elements generated considering the Douglas-Kroll relativistic effects, suitable for accurate spin-orbit coupling calculations." *J. Chem. Phys.* **2010**, *133*, 114107, 11 pages.

13. **T. Zeng**, D. G. Fedorov, and M. Klobukowski "Multireference study of spin-orbit coupling in the hydrides of the 6p-block elements using the model core potential method." *J. Chem. Phys.* **2010**, *132*, 074102, 15 pages.

12. **T. Zeng**, D. G. Fedorov, and M. Klobukowski "Model core potentials for studies of scalar-relativistic effects and spin-orbit coupling at Douglas–Kroll level. I. Theory and applications to Pb and Bi." *J. Chem. Phys.* **2009**, *131*,

124109, 17 pages.

11. **T. Zeng**, H. Mori, E. Miyoshi, and M. Klobukowski "Calibration of new model core potentials for main group elements." *Int. J. Quantum Chem.* **2009**, *109*, 3235-3245.

10. **T. Zeng** and M. Klobukowski "New model core potentials for gold." *J. Chem. Phys.* **2009**, *130*, 204107, 12 pages.

9. **T. Zeng** and M. Klobukowski "Relativistic model core potential study on the $Au^{+}Xe$ system." *J. Phys. Chem. A* **2008**, *112*, 5236-5242.

8. **T. Zeng**, Z. Jamshidi, H. Mori, E. Miyoshi, and M. Klobukowski "Electron affinities of heavier phosphoryl and thiophosphoryl halides APX_3 (A = O, S and X = Br, I)." *J. Comput. Chem.* **2007**, *28*, 2027-2033.

Institute of Coal Chemistry, Chinese Academy of Sciences

7. X.-D. Wen, **T. Zeng**, and H. Jiao 'Reply to "Comment on 'Density functional theory study of triangular molybdenum sulfide nanocluster and CO adsorption on it'" *J. Phys. Chem. B* **2006**, *110*, 14004-14005.

6. X.-D. Wen, **T. Zeng**, B.-T. Teng, F.-Q. Zhang, Y.-W. Li, and H. Jiao "Hydrogen adsorption on a $Mo_{27}S_{54}$ cluster: A density functional theory study." *J. Mol. Catal. A: Chemical* **2006**, *249*, 191-200.

5. C.-F. Huo, **T. Zeng**, Y.-W. Li, M. Beller, and H. Jiao "Switching end-on into side-on CN coordination: A computational approach." *Organometallics* **2005**, *24*, 6037-6042.

4. **T. Zeng**, X.-D. Wen, Y.-W. Li, and H. Jiao "Removal of surface sulfur from MoS_x cluster under CO adsorption." *J. Mol. Catal. A: Chemical* **2005**, *241*, 219-226.

3. X.-D. Wen, **T. Zeng**, Y.-W. Li, J. Wang, and H. Jiao "Surface structure and stability of MoS_x model clusters." *J. Phys. Chem. B* **2005**, *109*, 18491-18499.

2. **T. Zeng**, X.-D. Wen, Y.-W. Li, and H. Jiao "Density functional theory study of triangular molybdenum sulfide nanocluster and CO adsorption on it." *J. Phys. Chem. B* **2005**, *109*, 13704-13710.

1. **T. Zeng**, X.-D. Wen, G.-S. Wu, Y.-W. Li, and H. Jiao "Density functional theory study of CO adsorption on molybdenum sulfide." *J. Phys. Chem. B* 2005, *109*, 2846-2854.

Peer-Reviewed Book Chapters

2. **T. Zeng** and M. Klobukowski (2011) "Model core potential in the first decade of the XXI century." in *Practical Aspects of Computational Chemistry II, An Overview of the Last Two Decades and Current Trends*, J. Leszczynski and M. K. Shukla (Eds.), Springer, Chapter 8, 209-254 (PhD work).

1. **T. Zeng** and M. Klobukowski (2011) "Guide to Programs for Non-relativistic Quantum Chemistry Calculations." in *Handbook of Computational Chemistry*, J. Leszczynski (Ed.) Springer, Chapter 17, 611-630 (PhD work).

Programming

3. During my research in University of Waterloo, I implemented asymmetric top rotation into our in-house path-integral Monte Carlo program, MoRIBS-PIMC, and also parallelized the program. This program will be published in the near future. (PDF work).

2. During my visit to Iowa State University, I solely conceived the idea and wrote the program module of the *natural orbital analysis for the spin-orbit coupling configuration interaction wave function* in the worldwide famous program package GAMESS-US (PhD work).

1. During my visit to Iowa State University, I implemented our newly developed Douglas-Kroll Spin-Orbit Coupling Model Core Potential algorithm and all the potential and basis set libraries into GAMESS-US (PhD work).

Dissertations

2. PhD Thesis: Development and applications of model core potentials for the studies of spin-orbit effects in chemistry, 340 pages, submitted on November 26, 2010. (This thesis won the *Governor General's Gold Medal* of Canada.)

1. MSc Thesis: A Quantum Chemistry Study on CO Adsorption and Activation on Edges of Molybdenum Sulfide, 124 pages, published by Chinese Academy of Sciences, 2005.

Referee for Journals

1. Journal of Physics B: Atomic, Molecular & Optical Physics
2. Canadian Journal of Physics
3. Journal of Mathematical Chemistry
4. Chemical Physics
5. Theoretical Chemistry Accounts

Oral Presentations

14. **T. Zeng**, N. Ananth, and R. Hoffmann "Seeking small molecules for singlet fission: a heteroatom substitution strategy."
2014 Singlet Fission Workshop, June 21-24, Peaceful Valley, CO, USA

13. **T. Zeng** and P.-N. Roy "Superfluidity hidden in a forgotten corner."
Invited seminar at State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, December 12, 2013, Changchun, Jilin, China

12. **T. Zeng** and P.-N. Roy "Superfluidity hidden in a forgotten corner."
68th International Symposium on Molecular Spectroscopy June 17-21, 2013, Columbus, OH, USA

11. **T. Zeng** and P.-N. Roy "Superfluidity hidden in a forgotten corner."
96th Canadian Chemistry Conference and Exhibition May 26-30, 2013, Québec, QC, Canada

10. **T. Zeng**, H. Li, and P.-N. Roy "Asymmetric top rotations in superfluid *para*-hydrogen nano-clusters: the molecules with three buckets."
25th Canadian Symposium on Theoretical and Computational Chemistry July 22-27, 2012, Guelph, Ontario, Canada

9. **T. Zeng**, H. Li, and P.-N. Roy "Asymmetric top rotations in superfluid *para*-hydrogen nano-clusters."
67th International Symposium on Molecular Spectroscopy June 18-22, 2012, Columbus, OH, USA

8. **T. Zeng** "Spin-orbit coupling, model core potential, natural spinor, and some recent advances in microscopic superfluidity."
Invited seminar at State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, November 30, 2011, Changchun, Jilin, China

7. **T. Zeng**, H. Li, R. J. Le Roy, and P.-N. Roy "Adiabatic-hindered-rotor treatment of parahydrogen-water complex."
Applied Mathematics, Modeling and Computational Science Conference July 25-29, 2011, Waterloo, ON, Canada

6. **T. Zeng**, H. Li, R. J. Le Roy, and P.-N. Roy "Adiabatic-hindered-rotor treatment of parahydrogen-water complex."
MATRIX2011 July 10-15, 2011, Vancouver, BC, Canada

5. **T. Zeng**, H. Li, R. J. Le Roy, and P.-N. Roy "Adiabatic-hindered-rotor treatment of parahydrogen-water complex."
66th International Symposium on Molecular Spectroscopy June 20-24, 2011, Columbus, OH, USA

4. **T. Zeng**, D. G. Fedorov, M. W. Schmidt, and M. Klobukowski "Natural spinor: a new insight into spin-orbit coupling in chemistry."
Invited seminar at Department of Chemistry, University of Alberta, June 10, 2011, Edmonton, AB, Canada

3. **T. Zeng**, H. Li, R. J. Le Roy, and P.-N. Roy "Adiabatic-hindered-rotor treatment of parahydrogen-water complex."
Invited seminar at Department of Chemistry, University of Alberta, June 10, 2011, Edmonton, AB, Canada

2. **T. Zeng**, H. Li, R. J. Le Roy, and P.-N. Roy "Adiabatic-hindered-rotor treatment of parahydrogen-water complex."
94th Canadian Chemistry Conference and Exhibition June 5-9, 2011, Montreal, QC, Canada

1. **T. Zeng**, H. Li, R. J. Le Roy, and P.-N. Roy "Adiabatic-hindered-rotor treatment of parahydrogen-water complex." *11th Centre for Research in Molecular Modeling Symposium* June 4-5, 2011, Montreal, QC, Canada

Poster Presentations

13. **T. Zeng**, R. Hoffmann, and N. Ananth "The roles of pentacene electronic states in singlet fission, and more small chromophores"
American Conference on Theoretical Chemistry (ACTC) 2014, July 20-25, 2014, Telluride, CO, USA

12. **T. Zeng**, R. Hoffmann, and N. Ananth "The low-lying electronic states of pentacene and their roles in singlet fission."
2014 Singlet Fission Workshop, June 21-24, 2014, Peaceful Valley, CO, USA

11. **T. Zeng**, R. Hoffmann, and N. Ananth "The low-lying electronic states of pentacene and their roles in singlet fission."
4th New York Theoretical and Computational Chemistry Conference, March 21, 2014, Stony Brook, NY, USA

10. **T. Zeng**, G. Guillon, and P.-N. Roy "Asymmetric top rotors in superfluid *para*-hydrogen nano-clusters: the molecules with three buckets."
28th Symposium on Chemical Physics at the University of Waterloo November 2-4, 2012, Waterloo, ON, Canada

9. **T. Zeng**, H. Li, and P.-N. Roy "Superfluidity in pH_2 cluster with a water dopant."
Gordon Research Conference, Molecular & Ionic Clusters January 29- February 3, 2012, Ventura, CA, USA

8. **T. Zeng**, H. Li, and P.-N. Roy "Superfluidity in pH_2 cluster with a water dopant."
27th Symposium on Chemical Physics at the University of Waterloo November 4-6, 2011, Waterloo, ON, Canada

7. **T. Zeng**, D. G. Fedorov, M. W. Schmidt, and M. Klobukowski "Probing the L-S coupled wave function with the two-component natural spinors: algorithm, test, and examples."
51st Sanibel Symposium February 25 – March 1, 2011, St. Simons Island, GA, USA
(This poster won the *IBM-Löwdin Award*.)

6. **T. Zeng**, D. G. Fedorov, and M. Klobukowski "Model core potentials of p-block elements generated considering the Douglas-Kroll relativistic effects, suitable for accurate spin-orbit coupling calculations."
17*th Canadian Symposium on Theoretical Chemistry* July 25-30, 2010, Edmonton, AB, Canada
(This poster won the award of *Outstanding Poster Presenter*.)

5. **T. Zeng**, D. G. Fedorov, and M. Klobukowski "Model core potentials for studies of scalar-relativistic effects and spin-orbit coupling at Douglas–Kroll level. I. Theory and applications to Pb and Bi."
7th Canadian Computational Chemistry Conference July 20-24, 2009, Halifax, NS, Canada

4. **T. Zeng**, H. Mori, E. Miyoshi, and M. Klobukowski "Calibration of new model core potentials for main group elements."
91st Canadian Chemistry Conference and Exhibition May 24-28, 2008, Edmonton, AB, Canada

3. **T. Zeng** and M. Klobukowski "New families of model core potentials for gold."
91st Canadian Chemistry Conference and Exhibition May 24-28, 2008, Edmonton, AB, Canada

2. **T. Zeng** and M. Klobukowski "Relativistic model core potential study of the Au^+Xe system." *16th Canadian Symposium on Theoretical Chemistry* August 3-7, 2007, Memorial University of Newfoundland, St. John's, NL, Canada

1. **T. Zeng**, Z. Jamshidi, H. Mori, E. Miyoshi, and M. Klobukowski "Studies of APX_3 systems (A=O, S and X=Br and I)."
6th Canadian Computational Chemistry Conference July 26-30, 2006, University of British Columbia, Vancouver, BC, Canada

Teaching Experience

Period	Institute and Activity
2013.2	Department of Chemistry, University of Waterloo I taught Molecular Dynamics and Its Applications lectures as a substitute instructor for my supervisor.
2007.9	Department of Chemistry, University of Alberta I taught Advanced Computational Chemistry lectures as a substitute Instructor for my supervisor.
2005.9 – 2010.11	Department of Chemistry, University of Alberta I served as a teaching assistant in Introductory Chemistry and Atomic and Molecular Structure.