Lan Cheng

Department of Chemistry,
The Johns Hopkins University,
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Date of Birth: May 19, 1980

Education

- Ph.D. in Theoretical Chemistry, Peking University, China (Jul. 2009)

  Thesis: Four-component relativistic theory for NMR parameters (Sept. 2004 – Jul. 2009)
  Adviser: Professor Wenjian Liu

- B.S. in Chemistry, Tsinghua University, Beijing, China (Jul. 2001)

Working experience

- Assistant Professor, The Johns Hopkins University, Baltimore, USA (since Jan. 2016)

- Postdoctoral fellow, University of Texas at Austin, Austin, USA (Nov. 2011-Dec. 2015)
  Adviser: Professor John F. Stanton

- Postdoctoral fellow, University of Mainz, Mainz, Germany (Oct. 2009 – Oct. 2011)
  Adviser: Professor Jürgen Gauss

- Research assistant, Tsinghua University, Beijing, China (Sept. 2001 – Jun. 2004)
  Adviser: Professor Yadong Li

Research interests

- **Relativistic electronic-structure theory**

  Theoretical investigation of heavy-element containing systems requires accurate treatments of relativistic effects. My research deals with development of relativistic quantum-chemical methods for accurate computations of electric and magnetic properties for heavy-element compounds. The relativistic quantum-chemical machinery developed here are then applied in chemical and spectroscopic problems involving heavy elements.

- **Heavy-element chemistry and spectroscopy**

  Relativistic effects lead to unique electronic structure for heavy elements. Based on the relativistic quantum-chemical machinery, computational models are being developed for chemical and spectrocopic calculations of heavy-element compounds aiming at high accuracy.

List of publications:

Publications in peer-reviewed Journals

1. Y. Xiao, W. Liu, L. Cheng, and D. Peng, “Four-component relativistic theory for nuclear magnetic shielding constants: Critical assessments of different approaches”, J. Chem. Phys., **126**, 214101 (2007).

2. D. Peng, W. Liu, Y. Xiao, and L. Cheng, "Making four- and two-component relativistic density functional methods fully equivalent based on the idea of ‘from atoms to molecule’ ", J. Chem. Phys., **127**, 104106 (2007).

3. L. Cheng, Y. Xiao, and W. Liu, “Four-component relativistic theory for NMR parameters: Unified formulation and numerical assessments of different approaches”, J. Chem. Phys., **130**, 144102 (2009).

4. Q. Sun, W. Liu, Y. Xiao, and L. Cheng, “Exact two-component relativistic theory for nuclear magnetic resonance parameters”, J. Chem. Phys., **131**, 081101 (2009).

5. L. Cheng, Y. Xiao, and W. Liu, “Four-component relativistic theory for nuclear magnetic shielding: magnetically balanced gauge-including atomic orbitals”, J. Chem. Phys., **131**, 244113 (2009).

6. C. Puzzarini, G. Cazzoli, J. C. Lopez, J. L. Alonso, A. Baldacci, A. Baldan, S. Stopkowicz, L. Cheng, and J. Gauss, “Fourier-transform microwave and millimeter-wave spectroscopic investigation of CH_2FI guided by quantum-chemical calculations”, J. Chem. Phys. **134**, 174312 (2011).

7. L. Cheng and J. Gauss, “Analytical evaluation of first-order electrical properties based on the spin-free Dirac-Coulomb Hamiltonian”, J. Chem. Phys. **134**, 244112 (2011).

8. L. Cheng and J. Gauss, “Analytical energy gradients for the spin-free exact two-component theory using an exact block diagonalization for the one-electron Dirac Hamiltonian”, J. Chem. Phys. **135**, 084114 (2011).

9. W. Schwalbach, S. Stopkowicz, L. Cheng, and J. Gauss, “Direct perturbation theory in terms of energy derivatives: Scalar-relativistic treatment up to sixth order”, J. Chem. Phys. **135**, 194114 (2011).

10. L. Cheng and J. Gauss, “Analytic second derivatives for the spin-free exact two-component theory”, J. Chem. Phys, **135**, 244104 (2011).

11. S. Mao, L. Cheng, W. Liu, and D. Mukherjee, “A spin-adapted size-extensive state-specific multi-reference perturbation theory. I. Formal developments”, J. Chem. Phys. **136**, 024105 (2012).

12. S. Mao, L. Cheng, W. Liu, and D. Mukherjee, “A spin-adapted size-extensive state-specific multi-reference perturbation theory with various partitioning schemes. II. Molecular applications”, J. Chem. Phys. **136**, 024106 (2012).

13. C. Puzzarini, G. Cazzoli, J. C. Lopez, J. L. Alonso, A. Baldacci, A. Baldan, S. Stopkowicz, L. Cheng, and J. Gauss, “Rotational spectra of rare isotopic species of fluoroiodomethane: Determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations”, J. Chem. Phys., **137**, 024310 (2012).

14. L. Cheng, S. Stopkowicz, and J. F. Stanton, and J. Gauss, “The route to high accuracy in ab initio calculations of Cu quadrupole-coupling constants”, J. Chem. Phys. **137**, 224302 (2012).

15. S. Stopkowicz, L. Cheng, M. E. Harding, C. Puzzarini, and J. Gauss, “The bromine nuclear quadrupole moment revisited”, Mol. Phys. **111**, 1382 (2013).

16. R. Haunschild, L. Cheng, D. Mukherjee, and W. Klopper, “Communication: Extension of a universal explicit electron correlation correction to general complete active spaces”, J. Chem. Phys. **138**, 211101 (2013).

17. A. Le, T. C. Steimle, M. D. Morse, M. A. Garcia, L. Cheng, and J. F. Stanton, “Hyperfine interactions and electric dipole moments in the [16.0] 1.5(v=6), [16.0]3.5(v=7) and $X^2\Delta_{5/2}$ states of iridium monosilicide, IrSi”, J. Phys. Chem. A, **117**, 13292 (2013).

18. L. Cheng, J. Gauss, and J. F. Stanton, “Treatment of scalar-relativistic effects on nuclear magnetic shieldings using a spin-free exact-two-component approach”, J. Chem. Phys. **139**, 054105 (2013).

19. F. Wang, T. Steimle, A. Adam, L. Cheng, and J. F. Stanton, "The pure rotational spectrum of ruthenium monocarbide, RuC, and relativistic ab initio predictions", J. Chem. Phys. **139**, 174318 (2013).

20. L. Cheng, S. Stopkowicz, and J. Gauss, "Spin-free Dirac-Coulomb calculations augmented with a perturbative treatment of spin-orbit effects at the Hartree-Fock level", J. Chem. Phys. **139**, 214114 (2013).

21. M. C. McCarthy, L. Cheng, K. N. Crabtree, O. Martinez, Jr., T. L. Nguyen, C.C. Womack, and J. F. Stanton, "The simplest Criegee Intermediate (H_2C=O-O): Isotopic spectroscopy, equilibrium structure, and possible formation from atmospheric lightning", J. Phys. Chem. Lett. **4**, 4133 (2013).

22. L. Cheng, S. Stopkowicz, and J. Gauss, "Review: Analytic energy derivatives in relativistic quantum chemistry", Int. J. Quant. Chem. **114**,1108 (2014).

23. L. Cheng and J. Gauss, "Perturbative treatment of spin-orbit coupling within spin-free exact two-component theory", J. Chem. Phys., **141**, 164107 (2014).

24. R. Zhang, T. C. Steimle, L. Cheng and J. F. Stanton, "Permanent electric dipole moment of gold chloride, AuCl", Mol. Phys., **113,** 2073 (2015).

25. S. H. Southworth, R. Wehlitz, A. Picon, C. S. Lehmann, L. Cheng and J. F. Stanton, "Inner-shell photoionization and core-hole decay of Xe and XeF_2", J. Chem. Phys., **142**, 224302 (2015).

26. L. Cheng, J. Gauss, and J. F. Stanton, "Relativistic coupled-cluster calculations on XeF_6: Delicate interplay between electron-correlation and basis-set effects", J. Chem. Phys., **142**, 224309 (2015).

27. L. Cheng, "Benchmark calculations on the nuclear quadrupole-coupling parameters for open-shell molecules using non-relativistic and relativistic coupled-cluster methods", J. Chem. Phys., **143**, 064301 (2015).

28. X. Zhang, S. P. Sander, L. Cheng, V. S. Thimmakondu, and J. F. Stanton, "Matrix-isolated infrared absorption spectrum of CH2IOO radical", J. Phys. Chem. A, in press, DOI: 10.1021/acs.jpca.5b12143.

Book chapter(s)

1. A. Sen, L. Cheng, and D. Mukherjee, "Benchmark studies of spectroscopic parameters for hydrogen halide series via scalar-relativistic state-specific multireference perturbation theory", in *Concepts and Methods in Modern Theoretical Chemistry: Electronic Structure and Reactivity*, Edited by S. K. Ghosh and P. K. Chattaraj, CRC Press (2012).

Conference and seminar presentations:

Invited talks

1. "Cost-effective relativistic approaches for coupled-cluster methods", Coupled-cluster theory and related techniques, a satellite symposium of 14th ICQC, Boulder, CO, USA (2012).

2. "Cost-effective relativistic approaches based on spin separation", The VIIIth Congress of the International Society of Theoretical Chemical Physics, ISTCP-VIII, Budapest, Hungary (2013).

3. "Relativistic exact two-component coupled-cluster calculations of molecular properties", New Developments in Coupled-Cluster Theory, Telluride, CO, USA (2015).

Contributing conference talks and seminar presentations

1. "Four-component relativistic theory for NMR parameters", Chinese National Conference of Computational Chemistry, Nanjing University, China (2008).

2. "Unitary coupled-cluster linear response theory: Molecular applications for energy differences", Theoretical Chemistry Seminar, University of Heidelberg, Germany (2010).

4. "Analytic energy gradients in relativistic quantum chemistry: application of exact-two-component theory", 15th European Seminar on Computational Methods in Quantum Chemistry, Oscarsborg Fortress, Norway (2011).

5. “Relativistic theory for chemical shieldings: A spin-free exact two-component theory”, Southwest theoretical chemistry conference, Texas A&M University, TX, USA (2012).

6. “Recent advances in relativistic quantum chemistry”, Chemistry Seminar, Tsinghua University, China (2014).

7. “Ab initio calculation for the spin-orbit splittings of the nitrate radical (NO_3)”, 69th International Symposium on Molecular Spectroscopy, Champaign-Urbana, Illinois, (2014).

8. “High-accuracy ab initio calculation of metal quadrupole-coupling parameters”, 69th International Symposium on Molecular Spectroscopy, Champaign-Urbana, Illinois, (2014).

9. “Relativity throughout the periodic table”, Chemistry Seminar, Johns-Hopkins University, MD, USA (2014).

10. “Ab initio calculation on the photoelectron spectrum of methoxide”, 70th International Symposium on Molecular Spectroscopy, Champaign-Urbana, Illinois, (2015).

11. “New estimate of the copper nuclear quadrupole moment”, 70th International Symposium on Molecular Spectroscopy, Champaign-Urbana, Illinois, (2015).

Poster presentations

1. “Four-component relativistic theory for NMR parameters: Unified formulation of magnetic balance”, International Conference on Theory and Application of Computational Chemistry, TACC2008, Shanghai, China (2008).

2. “Four-component relativistic theory for NMR shielding tensors: Magnetically balanced gauge-including atomic orbitals”, The XIII Internatinal Congress of Quantum Chemistry, Helsinki, Finland (2009).

3. *“*Efficient treatments of relativistic effects in correlated methods”*,* Molecular Quantum Mechanics Conference 2010, University of California, Berkeley, CA (2010).

4. “Analytic energy derivatives in relativistic quantum chemistry”, The 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Waseda University, Tokyo, Japan (2011).

5. *“*Spin-free exact two-component theory for chemical shieldings”*,* 14th International Congress of Quantum Chemistry, Boulder, CO, USA (2012).