Selected Publications of Prof. Dr. Wenjian Liu

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1 Fundamentals of relativistic molecular quantum mechanics

1. *Handbook of Relativistic Quantum Chemistry*, ed. W. Liu (Springer, Berlin, 2017).
2. W. Liu*, *Big picture of relativistic molecular quantum mechanics*, Nat. Sci. Rev. **3**, 204 (2016).
3. R. Zhao, Y. Xiao, Y. Zhang, and W. Liu*, *Exact two-component relativistic energy band theory and application*, J. Chem. Phys. **144**, 044105 (2016).
4. W. Liu, *Effective quantum electrodynamics Hamiltonians: A tutorial review*, Int. J. Quantum Chem. **115**, 631 (2015); (E) 116, 971 (2016).
5. W. Liu*, *Advances in relativistic molecular quantum mechanics*, Phys. Rep. **537**, 59 (2014).
6. W. Liu*, *Perspective: Relativistic Hamiltonians*, Int. J. Quantum Chem. **114**, 983 (2014).
7. W. Liu* and I. Lindgren, *Going beyond 'no-pair relativistic quantum chemistry'*, J. Chem. Phys. **139**, 014108 (2013); (E) **144**, 049901 (2016).
8. W. Liu*, *Perspectives of relativistic quantum chemistry: The negative energy cat smiles*, Phys. Chem. Chem. Phys. **14**, 35 (2012).
9. W. Liu*, *The 'big picture' of relativistic molecular quantum mechanics*, in *Theory and Applications in Computational Chemistry: The First Decade of the Second Millenium*, AIP Conf. Proc. **1456**, 62 (2012).
10. W. Liu*, *Ideas of relativistic quantum chemistry*, Mol. Phys. **108**, 1679 (2010).
11. Z. Li, Y. Xiao, and W. Liu*, *On the spin separation of algebraic two-component relativistic Hamiltonians: Molecular Properties*, J. Chem. Phys. **141**, 054111 (2014).
12. Z. Li, Y. Xiao, and W. Liu*, *On the spin separation of algebraic two-component relativistic Hamiltonians*, J. Chem. Phys. **137**, 154114 (2012).
13. W. Liu* and D. Peng, *Exact two-component Hamiltonians revisited*, J. Chem. Phys. **131**, 031104 (2009).
14. D. Peng, J. Ma, and W. Liu*, *On the construction of Kramers paired double group symmetry functions*, Int. J. Quantum Chem. **109**, 2149 (2009).

15. 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).

16. W. Liu* and D. Peng, *Infinite-order Quasirelativistic Density Functional Method Based on the Exact Matrix Quasirelativistic Theory*, J. Chem. Phys. **125**, 044102 (2006); (E) **125**, 149901 (2006).

17. W. Kutzelnigg* and W. Liu*, *Quasirelativistic Theory Equivalent to Fully Relativistic Theory*, J. Chem. Phys. **123**, 241102 (2005).

2 Relativistic/nonrelativistic wave functions

1. Y. Lei, W. Liu* and M. R. Hoffmann*, *Further development of SDSPT2 for strongly correlated electrons*, Mol. Phys. **115**, 2696-2707 (2017).

2. C. Huang, W. Liu*, Y. Xiao, and M. R. Hoffmann, *iVI: an iterative vector interaction method for large eigenvalue problems*, J. Comput. Chem. **38**, 2481-2499 (2017).

3. A. Grofe, X. Chen, W. Liu, and J. Gao*, *Spin-multiplet components and energy splittings by multistate density functional theory*, J. Phys. Chem. Lett. **8**, 4838-4845 (2017).

4. P. Cassam-Chenaï*, B. Suo, and W. Liu*, *A quantum chemical definition of electron-nucleus correlation*, Theor. Chem. Acc. **136**, 52 (2017).

5. H. Li, W. Liu*, and B. Suo, *Localization of open-shell molecular orbitals via least change from fragments to molecule*, J. Chem. Phys. **146**, 104104 (2017).

6. Z. Cao, Z. Li*, F. Wang*, and W. Liu*, *Combining the spin-separated exact two-component relativistic Hamiltonian with the equation-of-motion coupled-cluster method for the treatment of spinCorbit splittings of light and heavy elements*, Phys. Chem. Chem. Phys. **19**, 3713 (2017).

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9. Z. Li, H. Li, B. Suo, and W. Liu*, *Localization of molecular orbitals: From fragments to molecule*, Acc. Chem. Res. **47**, 2758 (2014).

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11. Z. Li, S. Shao, and W. Liu*, *Relativistic explicit correlation: Coalescence conditions and practical suggestions*, J. Chem. Phys. **136**, 144117 (2012).

12. 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).

13. 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).

3 Relativistic properties

1. Y. Xiao, Y. Zhang, and W. Liu*, *Relativistic theory of nuclear spin-rotation tensor with kinetically balanced rotational London orbitals*, J. Chem. Phys. **141**, 164110 (2014).

2. Y. Xiao, Y. Zhang, and W. Liu*, *New experimental NMR shielding scales mapped relativistically from NSR: Theory and application*, J. Chem. Theory Comput. **10**, 600 (2014).

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6. Y. Xiao, Q. Sun, and W. Liu*, *Fully relativistic theories and methods for NMR parameters*, Theor. Chem. Acc. **131**, 1080 (2012).

7. 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).

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9. W. Kutzelnigg* and W. Liu*, *Relativistic theory of nuclear magnetic resonance parameters in a Gaussian basis representation*, J. Chem. Phys. **131**, 044129 (2009).

10. L. Cheng, Y. Xiao, and W. Liu*, *Four-component relativistic theory for NMR parameters: Unified formulation and numerical assessment of different approaches*, J. Chem. Phys. **130**, 144102 (2009); (E) **131**, 1 (2009).

11. 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).

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4 Time-dependent density functional theory

1. W. Liu* and Y. Xiao, *Relativistic time-dependent density functional theories*, Chem. Soc. Rev. **47**, 4481-4509 (2018).

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7. J. Liu, Y. Zhang, and W. Liu*, *Photoexcitation of Light-Harvesting C-P-C_{60} Triads: A FLMO-TD-DFT Study*, J. Chem. Theory Comput. **10**, 2436 (2014).

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9. Z. Li and W. Liu*, *Theoretical and numerical assessments of spin-flip time-dependent density functional theory*, J. Chem. Phys. **136**, 024107 (2012).

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5 Algorithms for large eigenvalue problems

1. C. Huang, W. Liu*, Y. Xiao, and M. R. Hoffmann, *iVI: an iterative vector interaction method for large eigenvalue problems*, J. Comput. Chem. **38**, 2481-2499 (2017); (E) **39**, 338 (2018).

6 The BDF package

1. W. Liu*, F. Wang, and L. Li, *The Beijing Density Functional (BDF) Program Package: Methodologies and Applications*, J. Theor. Comput. Chem. **2**, 257 (2003).

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