The Big Picture of Relativistic Molecular Quantum Mechanics

Wenjian Liu

College of Chemistry and Molecular Engineering, Peking University, Beijing, China

Relativistic Molecular Quantum Mechanics (RMQM) as the union of Relativistic Quantum Chemistry (RQC) and Quantum Electrodynamics (QED) consists of three components (Hamiltonian, wave function, and property), each of which is confronted with some fundamental issues, such as 'what is the appropriate relativistic Hamiltonian?'[1-8], 'how to make explicit and/or local representations of relativistic wave functions?'[9-13], 'how to formulate relativistic properties?'[14-16], 'how to interface RQC and QED?'[2-8], etc. In this lecture I shall try to address these fundamental issues from both conceptual and methodological standpoints, so as to establish the big picture of RMQM.

1. W. Liu, *Ideas of relativistic quantum chemistry*, Mol. Phys. **108** (2010) 1679.
2. W. Liu, *Perspectives of relativistic quantum chemistry: The negative energy cat smiles*, Phys. Chem. Chem. Phys. **14** (2012) 35.
3. W. Liu and I. Lindgren, *Going beyond `no-pair relativistic quantum chemistry'*, J. Chem. Phys. **139** (2013) 014108.
4. W. Liu, *Perspective: Relativistic Hamiltonians*, Int. J. Quantum Chem. **114** (2014) 983.
5. W. Liu, *Advances in relativistic molecular quantum mechanics*, Phys. Rep. **537** (2014) 59.
6. W. Liu, *Effective quantum electrodynamics Hamiltonians: A Tutorial Review*, Int. J. Quantum Chem. **115** (2015) 631.
7. W. Liu, Big picture of *relativistic molecular quantum mechanics*, Natl. Sci. Rev. **3** (2016) 204.
8. Handbook of Relativistic Quantum Chemistry, ed. W. Liu (Springer, 2017).
9. Z. Li, S. Shao, and W. Liu, *Relativistic explicit correlation: Coalescence conditions and practical suggestions*, J. Chem. Phys. **136** (2012) 144117.
10. Z. Li, H. Li, B. Suo, and W. Liu, *Localization of molecular orbitals: from fragments to molecule*, Acc. Chem. Res. **47** (2014) 2758.
11. W. Liu and M. R. Hoffmann, *SDS: the static-dynamic-static framework for strongly correlated electrons*, Theor. Chem. Acc. **133** (2014) 1481.
12. W. Liu and M. R. Hoffmann, *iCI: iterative CI toward full CI*, J. Chem. Theory Comput. **12** (2016) 1169.
13. Y. Lei, W. Liu, and M. R. Hoffmann, *Further development of SDSPT2 for strongly correlated electrons*, Mol. Phys. (2017, DOI: 10.1080/00268976.2017.1308029)
14. Y. Xiao, Q. Sun, and W. Liu, *Fully relativistic theories and methods for NMR parameters*, Theor. Chem. Acc. **131** (2012) 1080.
15. Y. Xiao and W. Liu, *Body-fixed relativistic molecular Hamiltonian and its application to nuclear spin-rotation tensor*, J. Chem. Phys. **138** (2013) 134104.
16. Y. Xiao, Y. Zhang, and W. Liu, *New experimental NMR shielding scales mapped relativistically from NSR: Theory and application*, J. Chem. Theory Comput. **10** (2014) 600.