

Theory

1. R. J. Bartlett and G. D. Purvis, "Many-body perturbation theory, coupled-pair many-electron theory and the importance of quadruple excitations for the correlation problem," Proceedings of the American Theoretical Chemistry Conference, Boulder, Colorado, Int. J. Quantum Chem. **14**, 561-581 (1978).
2. R. J. Bartlett and G. D. Purvis III, "Molecular applications of coupled cluster and many-body perturbation methods," Proceedings of the Nobel Symposium on Many-Body Theory, Lerum, Sweden, Physica Scripta **21**, 255-265 (1980).
3. G. D. Purvis, III and R. J. Bartlett, "A full coupled-cluster singles and doubles model: The inclusion of disconnected triples," J. Chem. Phys. **76**, 1910-1918 (1982).
4. L. Adamowicz, W. D. Laidig and R. J. Bartlett, "Analytical gradients for the coupled-cluster method," Int. J. Quantum Chem. Symp. **18**, 245-254 (1984).
5. Y. S. Lee, S. A. Kucharski and R. J. Bartlett, "A coupled cluster approach with triple excitations," J. Chem. Phys. **81**, 5906-5912 (1984).
6. J. Noga and R. J. Bartlett, "The full CCSDT model for molecular electronic structure," J. Chem. Phys. **86**, 7041-7050 (1987).
7. R. J. Bartlett, "Coupled-cluster approach to molecular structure and spectra: A step toward predictive quantum chemistry," J. Phys. Chem. (Feature Article) **93**, 1697-1708 (1989).
8. S. A. Kucharski and R. J. Bartlett, "The coupled-cluster single, double, triple and quadruple excitation method," J. Chem. Phys. **97**, 4282-4288 (1992).
9. J. F. Stanton and R. J. Bartlett, "The equation of motion coupled-cluster method. A systematic biorthogonal approach to molecular excitation energies, transition probabilities, and excited state properties," J. Chem. Phys. **98**, 7029-7039 (1993).
10. M. Nooijen and R. J. Bartlett, "A new method for excited states: Similarity transformed equation-of-motion coupled-cluster theory," J. Chem. Phys. **106**, 6441-6448 (1997).
11. N. Flocke and R. J. Bartlett, "A natural linear scaling coupled-cluster method," J. Chem. Phys. **121**, 10935 (2004).
12. R. J. Bartlett, V. F. Lotrich, I.V. Schweigert, "Ab initio DFT: The best of both worlds?" J. Chem. Phys. **123**, 062205 (2005).
13. A. Taube and R. J. Bartlett, "Frozen natural orbital coupled-cluster theory: Forces and applications to decomposition of nitroethane," J. Chem. Phys. **128**, 164101/1 – 164101/17 (2008).
14. R. J. Bartlett, "Towards an exact correlated orbital theory for electrons," Frontiers Article, Chem. Phys. Lett. **484**, 1-9 (2009).
15. M. Musial, A. Perera, and R. J. Bartlett, "Multireference coupled-cluster theory: The easy way," J. Chem. Phys. **134**, 114108/1-10 (2011).
16. P. Verma and R. J. Bartlett, "Increasing the applicability of density functional theory. III. Do consistent Kohn-Sham density functional methods exist?" J. Chem. Phys. **137**, 134102/1-12 (2012).
17. T. J. Watson, Jr., V. Lotrich, P. Szalay, A. Perera, and R. J. Bartlett, "Benchmarking for perturbative triple-excitations in EE-EOM-CC methods," J. Phys. Chem. A **117**, 2569-2579 (2013).