MAR16-2015-001644

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Multi-Configuration Pair-Density Functional Theory

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We have recently developed a new theoretical framework, called Multiconfiguration Pair-Density Functional Theory (MC-PDFT),[1] which combines multiconfigurational wave functions with a generalization of density functional theory (DFT). In this talk I will describe the basic principles of the theory and I present our latest results with MC-PDFT on spectroscopy,[2] charge-transfer systems[3] and molecules containing transition metals[4].

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[2] C. E. Hoyer, L. Gagliardi, and D. G. Truhlar, Multiconfiguration Pair-Density Functional Theory Spectral Calculations Are Stable to Adding Diffuse Basis Functions, *J. Phys. Chem. Lett.*, **(6), 2015**, pp 4184–4188

[3] S. Ghosh, A. L. Sonnenberger, C. E. Hoyer, D. G. Truhlar, and L. Gagliardi, Multiconfiguration Pair-Density Functional Theory Outperforms Kohn–Sham Density Functional Theory and Multireference Perturbation Theory for Ground-State and Excited-State Charge Transfer, *J. Chem. Theory Comput.*, **11 (8), 2015**, pp 3643-3649

[4] R. K. Carlson, D. G. Truhlar, and L. Gagliardi, Multiconfiguration Pair-Density Functional Theory: A Fully Translated Gradient Approximation and Its Performance for Transition Metal Dimers and the Spectroscopy of $Re_2Cl_8^{2-}$, *J. Chem. Theory Comput.*, **11 (9), 2015**, pp 4077-4085