Treating large-scale strong correlation in oligoacenes with adaptive configuration interaction and the driven similarity renormalization group

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Abstract

We have combined our adaptive configuration interaction (ACI) [J.B. Schriber and F.A. Evangelista, J. Chem. Phys. **144**, 161106 (2016)] with a density-fitted implementation of the second-order perturbative multireference driven similarity renormalization group (DSRG-MRPT2). We use ACI reference wave functions to recover static correlation for active spaces larger than the conventional CAS(18e, 18o) limit. The dynamical correlation is captured using the DSRG-MRPT2 to yield a complete treatment of electron correlation. We use the ACI-DSRG-MRPT2 to study the nature of strong correlation in extended oligoacenes, and demonstrate that we can use this method with the cc-pVTZ basis to affordably achieve sub kcal/mol accuracy with respect to experimental data.