

Abstract Submitted
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Residual Correlation Energies with Multi-Reference Density Functional Theory for Generalized Valence Bond Coupled-Cluster Methods KEITH LAWLER, Lawrence Berkeley National Lab, UC Berkeley, UC Davis, MARTIN HEAD-GORDON, UC Berkeley, Lawrence Berkeley National Laboratory — We consider the extension of single reference Kohn-Sham theory to the case of a Generalized Valence Bond-Coupled Cluster (GVB-CC) wave function acting as a multi-configuration auxiliary wave function for Kohn-Sham theory. GVB-CC methods account for only strong (static) correlations. Density functional theory (DFT) can be combined with the GVB-CC method to account for the missing residual (dynamic) correlation energy that is typically missing from a multi-configurational wavefunction method. We specifically look at the combination of DFT with the perfect pairing (PP) and coupled cluster valence bond (CCVB) methods. We also explore methods for polarizing the densities utilized by DFT to obtain the appropriate dissociation limit when spin-restricted versions of the GVB-CC methods are used.

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