Multireference Wavefunction Composite Strategies: From Main Group Species to the Transition Metals

Wanyi Jiang, Angela K. Wilson

Department of Chemistry and Center for Advanced Scientific Computing and Modeling (CASCaM), University of North Texas,
1155 Union Circle, #305070, Denton, Texas 76203-5017, U.S.A.

The *ab initio* correlation consistent Composite Approach (ccCA) is a thermochemical model devised to achieve energetics (i.e. enthalpies of formation, ionization potentials, proton affinities) akin to those obtained using electronic correlation methods such as CCSD(T) at the complete basis set limit, but as much greater computational efficiency. While the approach has proven to be of great utility, the prediction of features of potential energy surfaces, bond formation and bonding breaking, and excited states can warrant a multireference wavefunction-based approach. We describe developments towards the description of nondynamical electron correlation, via multireference composite strategies (MR-ccCA), efficient alternatives to such approaches, and diagnostics for the potential need for multireference wave function-based treatment.