Ab Initio Composite Methods: Beyond Ground State Main Group Species

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Ab initio composite methods provide a powerful means to address thermochemical properties of main group species. Despite their tremendous popularity, there has been limited application of these methods beyond ground state main group species. Several years ago, we introduced the correlation consistent Composite Approach (ccCA) as an approach that was not only able to address main group chemistry, but also could address transition metal chemistry. A similar algorithm of multireference methods, the multireference correlation consistent Composite Approach (MR-ccCA), was developed to address problems for which a single reference wavefunction may not be suitable, such as for excited states and bond formation and dissociation. As well, because of the synergy of the steps within MR-ccCA, the method has been effective in the prediction of potential energy surfaces.

Recent developments for ccCA and MR-ccCA are discussed, including developments and successes for transition metal chemistry, where ccCA provides a powerful gauge of the performance of density functional approaches, particularly in the absence of experimental data.

Over 200 transition metals species have been investigated, and over a thousand main group species have been investigated, ranging from weakly to tightly bound systems. Overall, ccCA is one of the most effective *ab initio* composite methods available.