Quantiative Modeling across the Periodic Table

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Computational chemistry provides a viable way to address a wide range of chemistry that is difficult or cost-prohibitive to evaluate by other means – from the description of short-lived excited states, to the understanding of complex interactions. *Ab initio* computational chemistry approaches have become an invaluable aid in the quantitative prediction of kinetic and thermodynamic properties, enabling "chemical accuracy" – typically defined as ± 1 kcal/mol or less from reliable experiment for energetic properties – to be possible. This level of accuracy, however, is limited predominantly to small molecules comprised of no more than ~2-10 main-group atoms, as computational cost - the amount of CPU time, memory, and disk space required for a calculation - quickly grows as the molecule size increases, and, as the sophistication of the methodology utilized increases.

A variety of developments have resulted in less computationally costly methods that still allow a high level of accuracy to be achieved. Such methods bring the promise of application to larger and more experimentally relevant chemical problems. Among the most widely used approaches are composite methods, methods which mimic the accuracy of expensive and often computationally intractable electronic structure computations using additive approximations obtained from multiple computations of higher efficiency and lower accuracy. Unfortunately, overall, many composite methods are still plagued with problems such as high computational cost, required modifications for different portions of the periodic table (e.g., s-block elements), inability to address transition metal species, and/or significant parameterization. We have developed a composite method, the correlation consistent Composite Approach, which can be used throughout the periodic table without modification, does not require parameterization, and does address the thermochemistry of metal complexes.