

Effective (and Ineffective) Quantum Chemistry Strategies for Transition Metals and Beyond

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Achieving quantitative accuracy in the prediction of energetic properties can become challenging for transition metal species due to increasing computational costs and, often, increasing molecular complexity. The challenges become even more substantial for the lanthanides and actinides. Developments by our group and applications that have provided insight about both energetic predictions for species of the lower part of the periodic table and the theoretical strategies used for the predictions (i.e., density functional approximations, and *ab initio* single and multi-reference strategies) will be highlighted. Specifically, the correlation consistent Composite Approach (ccCA), which effectively has been utilized for many hundreds of main groups species, will be discussed, focusing upon recent efforts for transition metal and heavy element chemistry. Density functional approaches will also be discussed.