Accurate and Efficient Treatment of Heavy Elements with Multireference Correlation Consistent Composite Approach (MR-ccCA)

Yifan Jin and Angela K. Wilson

Department of Chemistry, Michigan State University, East Lansing, MI 48824

This presentation focuses on the principles of the multireference correlation consistent Composite Approach (MR-ccCA) and its application to the molecules with transition metals. Accurate computation of the chemical and physical properties of the heavy elements especially the transition metal systems is a great challenge for theoretical chemists. One of the difficulties is that many of these systems have strong multireference character, and thus the single-reference *ab initio* methods such as coupled-cluster theory may not be capable of predicting the properties of these systems with enough accuracy. And the high-level multireference methods with large basis set are mostly computationally prohibitive especially the effects that are essential to the accuracy such as core-core/core-valence coupling, spin-orbit coupling, and scalar relativistic correction are taken into account. The basic idea of MR-ccCA is to emulate the high-accuracy but expensive methods by compositing a series of computationally efficient multireference approaches. This method has been applied to the main group elements, and the results indicate that it could reach the same accuracy as the more complicated multireference methods but significantly reduce the computational costs. However, it has never been used to study the molecules with transition metals. Since the multireference character for transition metal compounds is much more significant, the MR-ccCA is expected to be a powerful method for such systems. But due to the complexity of such molecules, the formula proposed previously needs to be modified to ensure the accuracy. Here we will present the new MR-ccCA method that could accurately and efficiently predict the various properties of the heavy elements. The method itself will be systematically introduced, and the results of the benchmark calculations will be presented.