WESTERN MICHIGAN UNIVERSITY
College of Arts and Sciences
Department of Chemistry

The Department of Chemistry

Presents

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Thermodynamic Predictions: Effective (and Ineffective) Computational Strategies across the Periodic Table

Abstract:

In the rational analysis and design of molecular species, energetic data is often the most critical information needed. One of the longstanding challenges in computational chemistry, however, is in achieving accurate energetics (i.e., enthalpies of formation, ionization energies) for molecules species across the periodic table, and for molecules of increasing size. Challenges that can be encountered include limited experimental gauges for calculations, computational (i.e., computer memory, disk space, and CPU time) limitations, and, often, increasing atomic and molecular complexity beyond the first rows of the periodic table. Strategies for addressing these challenges and predicting quantitatively accurate energies will be discussed. The importance of the choice of thermochemical pathway, effective gauges and insight into computational approaches, particularly for transition metal species and heavy element species will be discussed, as will ground state and excited state species.

Monday October 8, 2018
4:00 pm
Chemistry Building, Room 1220