

Departmental Colloquium

Friday, October 27, 2017, 4:00 pm
Seeley G. Mudd (SGM) Room 101

Professor Angela Wilson

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Accurate (and Inaccurate) Energetic and Spectroscopic Properties 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 achieving accurate energetics (i.e., enthalpies of formation, ionization energies) for molecules species across the periodic table, and for molecules of increasing size. Common challenges include limited experimental gauges for calculations, computational limitations (i.e., computer memory, disk space, and CPU time), 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. Other topics will include the importance of selecting the thermochemical pathway; effective gauges and insight into theory, particularly for transition metal species; heavy element species; and ground-state and excited-state species.

Hosted by Professor Anna Krylov

The scientific community is invited