Tuesday, November 14, 2017, 12:30 pm
Seaver Science Auditorium, Room 150
SSC Auditorium next to the library

Professor David Dixon

Department of Chemistry
The University of Alabama

Recent Advances in Computational Inorganic Chemistry: Actinides, Metal Oxides, and MOFs

Abstract:

Modern computational chemistry methods on advanced computer architectures are now capable of predicting the properties of inorganic compounds not only qualitatively but also quantitatively. This talk will describe such applications for actinides, metal oxides, and MOFs, using a range of computational electronic structure approaches. The formation of AnO_2^+ ions and their reactions with water molecules will be described including proposed novel structures, which depend on the periodic behavior of the actinides. The periodic properties of AnF_x and $An(OH)_y$ will also be discussed including electron affinities, ionization energies, fluoride affinities, and bond dissociation energies. The reactivity of transition metal oxides with water, alcohols, and acid gases will be described with a focus on their potential for catalysis and their Lewis and Brönsted acid-base chemistry as well as redox properties. The growth of metal oxide nanoclusters will be described including how clustering energies can be used to estimate energetic properties of the bulk. Acid gases, including CO_2, play an important role in a range of large-scale energy applications. The interactions of acid gases with models of MOF-2 will also be described. The goal of the talk is to show how computational electronic structure methods can be used to provide unique insights into the chemical properties of inorganic species. This work is supported by the U.S. Department of Energy Office of Science, Basic Energy Sciences.

Hosted by Professor Karl Christe

The scientific community is invited

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