TCI SEMINAR

Predicting Molecular Crystal Properties with Quatum Chemistry

Monday, October 29, 2012
3:00 p.m. Room 8335

Professor Gregory Beran

Department of Chemistry
University of California-Riverside

Molecular crystal structure affects the bioavailability of pharmaceuticals, the charge carrier efficiency of organic semiconductors, the products of solid-state reactions, and the explosive performance of energetic materials. Because different packing arrangements, or polymorphs, are often very close in energy, predicting molecular crystal properties from first principles is extremely difficult. We have developed a new, fragment-based quantum/classical hybrid model that makes it possible to apply high-level electronic structure methods to molecular crystal structure prediction. This model treats intramolecular effects and short-range pairwise intermolecular interactions quantum mechanically, while longer-range and many-body interactions are approximated classically. This model makes it possible reproduce experimental crystal structures and to predict small-molecule crystal lattice energies to within experimental accuracy. We will examine its performance in interesting polymorphic crystals such as aspirin and oxalyl dihydrazide.

Theoretical Chemistry Institute Seminar Series