Exploration and learning of free energy landscapes of molecular crystals and oligopeptides

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Theory, computation, and high-performance computers are playing an increasingly important role in helping us understand, design, and characterize a wide range of functional materials, chemical processes, and biomolecular/biomimetic structures. The synergy of computation and experiment is fueling a powerful approach to address some of the most challenging scientific problems. In this talk, I will describe the efforts we are making in my group to develop new computational methodologies that address specific challenges in free energy exploration and generation. In particular, I will describe our recent development of enhanced free energy based methodologies for predicting structure, polymorphism, and defects in atomic and molecular crystals, for exploring first-order phase transitions, and for determining conformational equilibria of oligopeptides. The strategies we are pursuing include large time-step molecular dynamics algorithms, heterogeneous multiscale modeling and learning techniques, which allow "landmark" locations (minima and saddles) on a high-dimensional free energy surface to be mapped out, and temperature-accelerated methods, which allow relative free energies of the landmarks to be generated efficiently and reliably. I will then discuss new schemes for using machine learning techniques to represent and perform computations using multidimensional free energy surfaces. Finally, if time permits, I will describe the use of machine learning techniques to enhance the accuracy and efficiency of density functional theory calculations based on density learning models.