Enhanced free energy based structure prediction in materials science

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Abstract:
Theory and computation, in synergy with experiment, are playing an increasingly important role in the design and characterization of new materials. In this talk, I will describe the efforts we are making in my group to develop new computational methodologies that address specific challenges in materials modeling. In particular, I will describe our recent development of enhanced free energy based methodologies for predicting structure and polymorphism in molecular crystals [1,2] and for determining conformational equilibria of oligopeptides [3-6]. The strategies we are pursuing include heterogeneous multiscale modeling 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. Results from applications to small, bound peptides and various atomic and molecular crystals, including one of the targets from the recent CCDC sixth blind structure prediction test, and co-crystals will be presented. I will also discuss the application of our computational protocol in the study of first-order phase transitions. Finally, future directions and challenges will be highlighted [7,8].

References:

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8. “Simulating long-time behavior of materials: A case study of the melting of a solid”, A. Samanta and M. E. Tuckerman *Phys. Rev. X* (submitted).