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Materials *in silico*: Structure, transport, and functionalization

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Theory and computation are playing an increasingly important role in design and characterization of new materials. In its description of the Materials Genome Initiative, the National Science and Technology Council called for an integrative approach to materials discovery and development involving a synergy between theory/modeling, experimentation, and engineering. In this talk, I will describe the efforts we are making in my group to develop new computational methodologies and address specific applications in materials chemistry. Specifically, I will outline our strategy for enhancing sampling of conformational equilibria in complex systems and demonstrate its performance in the prediction of polymorphism in molecular crystals. I will also review our work employing *ab initio* molecular dynamics in the study of proton transport in various hydrogen bonded media, including water Finally, I will discuss out recent efforts to understand and design new functionalizations of semiconductor surfaces through the creation of organic/semiconductor interfaces.