Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Atomistic simulations of materials chemistry: from nanoelectronics to energetic materials

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ABSTRACT

Predictive, physics-based modeling with quantified uncertainties has the potential to revolutionize the design and certification of materials and devices. Accomplishing this requires not only advances in modeling and simulation across scales, but also their synergistic combination with experiments via rigorous methods to quantify uncertainties and arrive at the desired decision in an optimal manner. I will illustrate our recent progress in the field with two applications:

Atomistic simulations of electrochemical reactions. I will describe a method that combines reactive interatomic potentials with a modified charge equilibration method to simulate electrochemical cells of interest in nanoelectronics and energy. We apply the method to electrometalization cells on interest for nonvolatile memory applications. These resistance-switching devices operate via the electrochemical formation and disruption of metallic filaments and our simulations predict switching timescales ranging from hundreds of picoseconds to a few nanoseconds for device dimensions corresponding to the scaling limit. The simulations provide the first atomic-scale picture of the operation of these devices and show that stable switching proceeds via the formation of small metallic clusters and their progressive chemical reduction as they become connected to the cathode.

Molecular dynamics chemical reactions under extreme conditions. We use reactive force fields to characterize chemical reactions in high-energy density materials under dynamical mechanical and electromagnetic insults. Under such conditions chemical reactions can occur under nonequilibrium conditions and our goal is to understand and, eventually, exploit such chemistry.

The impact of predictive simulations in materials design would be enormously accelerated if advanced simulation tools were universally available and useful. I will describe nanoHUB.org, a web-portal that provides users from around the world access to simulation tools free of charge and simply using a web-browser, with no need to download and install any software or provide hardware resources. I will illustrate the use of online materials simulations for research and education.