6b Multiscale Modeling of Materials Properties and Function

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Multiscale modeling has emerged over the past decade as a powerful, integrated computational approach for understanding, analyzing, and quantitatively predicting the behavior of complex systems. Fundamental research in the field has addressed the need for establishing rigorous links between different theoretical formalisms over widely different space and time scales. Significant progress has been made in the prediction of macroscopic behavior driven by atomic- and/or microstructural-scale mechanisms, acceleration of the dynamics of infrequent events, as well as bifurcation analysis of complex systems that require atomic- or microscopic-scale description. In this presentation, I will focus on electronic material systems, such as thin-film and nanostructured forms of metallic and semiconductor materials that are used commonly in the fabrication of electronic, optoelectronic, and photovoltaic devices. The function of these materials depends strongly on their structure and resulting properties. The prediction of relationships between the processing, structure, and function of such materials has been a long-standing theoretical and computational challenge in materials science and engineering and has driven the development of a broad class of multiscale modeling methods. Specifically, I will discuss in detail some recent contributions toward addressing problems of structural transitions, surface reactivity & roughness, and mechanical reliability of technologically important electronic materials. This work motivates system-level understanding powered by microscopic stochastic or deterministic descriptions. In this context, the potential for developing a “global” framework capable of performing system-level analysis through first-principles-based microscopic simulation will be emphasized. Toward this end, I will discuss recent advances in developing coarse time-stepper-based approaches to enable atomistic simulations of long-time dynamics and bifurcation & stability analyses.