Title: Development and Application of Interatomic Potentials for Heterogeneous Nanostructures

Type: Faculty & Graduate Student

Awardee: Scott Dunham & Graduate Student

Mentors: Scott Dunham – UW; Anter El-Azab – PNNL

Description: The focus of the proposed project is on the development of accurate empirical interatomic potentials for heterogeneous materials systems. We propose to develop potentials that can be successfully applied across multiple phases and (most critically) at materials interfaces. We will specifically explore potentials that account for charge transfer between atoms to allow for the potential to span interfaces among metallic, ionic and covalently bonded systems. The aim is to generate an approach that is applicable across a broad array of material systems. In addition to the potential development, the work will include use of density functional theory (DFT) calculations for calibration and molecular dynamics (MD) simulations as a tool for applications. Specific material systems of initial focus will include doped Si/SiO_2 interfaces and transition metal/metal oxide interfaces. The potentials will be applied to applications in nanotechnology and nanoelectronics, specifically the development of modeling tools for the fabrication of Nanoscale silicon transistors and metal/metal-oxide nanostructures. The work will involve collaboration between the Nano/Microtechnology Modeling Laboratory at UW and the Theory, Modeling & Simulation Group at PNNL.