

MAR13-2012-020237

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Mechanistic Design of New Materials and Processes through Multifunctional Atomic-Scale Simulations
SUSAN SINNOTT, University of Florida

Multifunctional systems that contain heterogeneous interfaces are ubiquitous in numerous applications, including catalysis, electronic devices, friction, and coatings. Traditionally, computational studies of these complex interfacial systems have relied on methods such as first-principles density functional theory (DFT), because of the difficulty in describing the changes in bonding environment with empirical approaches. Here, empirical, charge optimized many-body (COMB) potentials are used in classical, atomic-scale simulations to examine several model systems that involve heterogeneous material interfaces or surface reactions at size scales that are much larger than are currently tractable with traditional DFT methods. . The COMB potentials allow for dynamic charge transfer between atoms and across interfaces, and are demonstrated to describe metallic, covalent, and ionic bonding across interfaces and at surfaces. The simulations yield mechanistic insights that allow for the design of materials and optimization of process conditions for several applications, including catalysis, thin-film growth, and supported two-dimensional materials with well-defined interfacial interactions.