Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Simulation of complex materials structures with charge optimized many-body potentials

Phillpot, Simon, sphil@mse.ufl.edu, University of Florida

ABSTRACT

Many device structures combine the functionality of materials with very different bonding types: metallic, ionic, and covalent. Traditional empirical potentials have been designed to consider one type of bonding only. The Charge Optimized Many-Body (COMB) approach allows for the seamless simulation of structures composed of dissimilar materials. This is because COMB includes a charge equilibration method that allows each atom to autonomously and dynamically determine its charge, and a sophisticated description of bond order, by which the strength of an individual pair bond is modulated by the presence and strength of other local bonds. Simulations using COMB potentials are orders of magnitude faster than electronic-structure calculations, can consider much larger systems, and can easily simulate dynamically behavior. The power of this approach is illustrated from problem of interest for various condensed phase systems including U/UO_2, Zr/ZrO_2, and Cu/SiO_2.