Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Charge-Flow Regulation at Material Interfaces in Atomistic Models[1] STEVEN VALONE, Los Alamos National Laboratory — An important class of materials problems of great interest consists of composites of metals and metal oxides. At sharp metal/metal oxide interfaces, the oxygen concentration is varying radically over short distances. For this reason, at the atomistic level, variable-charge atomistic models are required that control charge flow at these interfaces. Charge flow is controlled through chemical potential equalization among its constituents. Existing models of chemical potential, such as the Iczkowski-Margrave (IM) model, are linear in the charge as is appropriate for metals. Here a new, "fragment" model Hamiltonian is constructed at the atomistic level commensurate with the IM model, as opposed to the one-electron model Hamiltonians that underlie tight-binding and related methods. Essential properties of the fragment model Hamiltonian include an alternative charge dependence compared to the IM model, charge-flow regulation, absent in the IM model, preservation of a sense of covalent-ionic balance, and capture of important theoretical limits.

[1]Support from the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number 2008LANL1026, is acknowledged.

Steven Valone
Los Alamos National Laboratory

Date submitted: 19 Nov 2010 Electronic form version 1.4