Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density Functional Atom-In-Molecule Force Field for Charge Transfer Systems[1] SUSAN R. ATLAS, Department of Physics and Astronomy, University of New Mexico, STEVEN M. VALONE, Materials Science and Technology Division, Los Alamos National Laboratory — Given an arbitrary molecular structure and corresponding total electronic density, the Hohenberg-Kohn theorem of density functional theory induces an approximate but unique atom-in-molecule density decomposition [1]. The decomposition is expressed as an ensemble-of-ensembles, a weighted double sum over ionic and excited state densities, and yields effective atomic charges consistent with chemical intuition, and in remarkable accord with the topological AIM theory of Bader. We show that this decomposition further induces a corresponding ensemble energy expression and multiscale force field appropriate for open, charge-transfer dynamical systems simulation. [1] SR Atlas, J Dittman, V Janardhanam, G Amo-Kwao, and SM Valone, to be submitted (2013).

[1]Supported by DTRA CB Basic Research Grant HDTRA1-09-1-0018.

Susan R. Atlas
Department of Physics and Astronomy, University of New Mexico

Date submitted: 15 Nov 2013 Electronic form version 1.4