Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density-Decomposed Orbital-Free Density Functional Theory for Covalent Systems and Application to Li-Si alloys[1] JUNCHAO XIA, EMILY CARTER, Princeton Univ — We propose a density decomposition scheme using a Wang-Govind-Carter (WGC)-based kinetic energy density functional (KEDF) to accurately and efficiently simulate covalent systems within orbital-free (OF) density functional theory (DFT). By using a local, density-dependent scale function, the total density is decomposed into a localized density within covalent bond regions and a flattened delocalized density, with the former described by semilocal KEDFs and the latter treated by the WGC KEDF. The new model predicts reasonable equilibrium volumes, bulk moduli, and phase ordering energies for various semiconductors compared to Kohn-Sham (KS) DFT benchmarks. The surface energy of Si(100) also agrees well with KSDFT. We further apply the model to study mechanical properties of Li-Si alloys, which have been recently recognized as a promising candidate for next-generation anodes of Li-ion batteries with outstanding capacity. We study multiple crystalline Li-Si alloys. The WGCD KEDF predicts accurate cell lattice vectors, equilibrium volumes, elastic moduli, electron densities, alloy formation and Li adsorption energies. Because of its quasilinear scaling, coupled with the level of accuracy shown here, OFDFT appears quite promising for large-scale simulation of such materials phenomena.

[1]Office of Naval Research, National Science Foundation, Tigress High Performance Computing Center

Junchao Xia
Princeton Univ

Date submitted: 14 Nov 2013 Electronic form version 1.4