

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

A linear scaling ab initio study of impurities and the metal-insulator transition in doped silicon¹ YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, CONRAD MOORE, Department of Physics, Louisiana State University, MARKUS EISENBACH, Oak Ridge National Laboratory, YI ZHANG, KA-MING TAM, MARK JARRELL, Department of Physics, Louisiana State University — Impurities in silicon are responsible for the states in the band gap, and they play a key role in modulating the conductivity of semiconductor devices. In this presentation, we discuss our computational efforts to investigate the metal-insulator transition of these states, particularly, in Titanium- and Sulfur- doped silicon. Both are potential highly efficient photovoltaic materials and are also targeted materials for the study of Mott and Anderson localization. We introduce a supercell scaling ansatz to identify the transition and validate it on the single-band Anderson model. We then apply the locally-self consistent multiple scattering (LSMS) method to the calculation and characterization of these mid-gap states. The LSMS method is a linear scaling ab initio method based on real space multiple scattering theory and Green function technique, and is one of the few scientific application codes capable of demonstrating performance beyond the petascale. To accurately describe the single impurity states, we employ large unit cells with more than 10,000 atomic sites.

¹This work is supported in part by NSF/XSEDE ECSS program

Yang Wang
Pittsburgh Supercomputing Center, Carnegie Mellon University

Date submitted: 11 Nov 2016

Electronic form version 1.4