Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Diffusion Monte Carlo Calculations of Formation Energies of Charged Self Interstitial Defects in Silicon[1] JONATHAN L. DUBOIS, DANIEL ABERG, VINCENZO LORDI, Lawrence Livermore National Lab — Scattering and trapping of carriers by charged point defects represent a significant limiting factor on carrier lifetimes in semiconductors. Given that long carrier lifetimes are essential for a wide range of semiconductor applications, accurate methods for predicting defect concentrations and defect-induced intragap energy levels are needed. Previous studies of neutral defects in silicon show significant deviations between DFT and Diffusion Monte Carlo (DMC) benchmark calculations of formation energies. Here we present DMC results for the formation energies of charged self interstitial defects in bulk silicon and extract charge state transition energy levels, which we compare to DFT LDA and hybrid functional results.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344.

Jonathan L. DuBois
Lawrence Livermore National Lab

Date submitted: 11 Dec 2009 Electronic form version 1.4