Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A Metal-Insulator Transition in Silicon Hyperdoped with Chalcogens ELIF ERTEKIN, MARK WINKLER, MIT, AURORE SAID, MICHAEL AZIZ, Harvard, TONIO BUONASSISI, JEFFREY GROSSMAN, MIT — Hyperdoped Silicon, the material resulting from the laser doping of Silicon to impurity concentrations orders of magnitude beyond the room temperature solubility limit, can exhibit unique properties. For example, "Black Silicon", formed from laser doping with chalcogens S, Se, or Te, exhibits anomalous sub band gap optical absorption at photon energies as low as 0.5 eV and a flat absorption spectrum. While this has piqued interest in the use of Black Silicon for optoelectronics and photovoltaics, there has not yet been a clear explanation for the enhanced optical properties. Focusing on the Se doped systems, we use Density Functional Theory to show that the optical absorption results from an impurity induced insulator to metal transition. Our calculations indicate that an isolated Se impurity introduces a localized electronic state in the band gap. At higher defect concentrations, the transition to the metallic state is demonstrated by an increase in the defect level bandwidth and the eventual merging of the defect state with the conduction bands. The concentration at which this occurs corresponds very well with experimental low temperature Hall effect measurements.

Elif Ertekin
Massachusetts Institute of Technology

Date submitted: 19 Nov 2010 Electronic form version 1.4