

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Hybrid functional calculations of Copper impurities and related complexes in Silicon ABHISHEK SHARAN, Department of Physics and Astronomy, University of Delaware, Newark DE 19716, ZHIGANG GUI, ANDERSON JANOTTI, Materials Science and Engineering, University of Delaware, Newark DE 19716 — Copper impurities affect electronic and optical properties of semiconductors. Cu is an ubiquitous impurity and can be introduced unintentionally during various processing step. In silicon, the fast-diffusing interstitial Cu donor often passivates shallow-acceptor dopants, affecting the electronic characteristics of devices, while deep levels associated with other forms of the Cu impurity degrade device performance. Here we revisit the problem of the Cu impurity in Si using first principles calculation based on a hybrid functional. We discuss the relative stability of the substitutional and interstitial forms, as well as the formation of complexes with hydrogen and oxygen impurities. The results of our calculations will be compared with recent experiments on the electrical activity of Cu impurities in Si.

Abhishek Sharan
Department of Physics and Astronomy, University of Delaware, Newark DE 19716

Date submitted: 04 Nov 2015

Electronic form version 1.4