

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**A first principles study of the localized electronic states of noble metal atoms doped in Si nanocrystals** CEDRIC L. MAYFIELD, University of Texas at Arlington, M. SAIF ISLAM, University of California-Davis, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboratory, MUHAMMAD N. HUDA, University of Texas at Arlington — The quest for a efficient energy conversion material has necessitated a detail study of semiconductors. Silicon is already playing important roles in many useful nano-applications. To optimize these nano-applications, electronically tailored nano-materials are needed. A number of semiconductor nano-materials are synthesized using metal as catalysts contributing to various impurities into the nanomaterials. The solubility of a metal in nanomaterials is significantly higher than that in bulk materials. In this presentation, electronic and structural properties of noble metal atoms doping in silicon nano-crystals will be explored using density functional theory. The pristine nanocrystals are based on three different isomers of bulk silicon. We have identified the lower energy isomer and doped it with noble metals. Characterization of the structural changes is accomplished by studying the bonding near the impurity as a function of dopant site. Furthermore, energetic of these nano-structures, both doped and un-doped, such as binding energies, formation energies, and HOMO LUMO gaps will be compared along with their charge densities to identify localizations with respect to impurity site. Magnetism and surface terminations will also be addressed.

Muhammad Huda  
Department of Physics, University of Texas at Arlington

Date submitted: 29 Dec 2010

Electronic form version 1.4