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Structural and Optical Properties of Amorphous and Crystalline Silicon Surfaces with Silver Adsorbates

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The optical properties of silicon surfaces are affected by their atomic structure and in particular by whether their lattice is crystalline or amorphous [1]. The modeling of amorphous structures is challenging because they are thermodynamically metastable and must be characterized by short range atomic order. We have developed a procedure which starts with molecular dynamics simulation of crystalline silicon (c-Si), followed by simulated thermal quenching using ab-initio electronic structure calculations. The pair correlation function for both a-Si and c-Si are compared regarding their structural properties [2]. The optical properties of these structures are investigated using density functional theory with the VASP software package [3]. Density of electronic states, band gap and intensity of light absorption with and without silver adsorbates are presented. These calculations are further extended to study the photovoltaic properties of Si surfaces in terms of the reduced density matrix. The surface photovoltage (SPV) created by steady light absorption and charge redistribution is calculated for Si slabs containing one or three adsorbed Ag atoms. Our results are compared with previous theoretical [4] and experimental results. New results show that silver adsorbates increase SPV at lower photon energies for both a-Si and c-Si. The SPV also increases with the thickness of the silicon slab.

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