Optical properties of the $Si(111) : H$ surface with adsorbed Ag clusters

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Systems composed of Ag clusters adsorbed on the $Si(111) : H$ surface have been computationally studied with density functional (DFT) and time-dependent DFT methods, to obtain their optical properties. The systems have been modeled as slabs with increasing number of layers, and increasing number oif Ag atoms in the clusters. Using codes in the VASP [1] and Gaussian03 [2] packages, calculations have provided atomic conformations, HOMO-LUMO excitation energies, electron binding energies, and electronic oscillator strengths. Results are presented for the correlation between these properties and the size of the systems. Analyses of the results provide insight on trends relevant to the absorption of near IR, visible, and near UV light, of interest in measurements of photovoltages [3], and in the utilization of solar energy.

1. J. Hafner, J. Comput. Chem. **29**, 2044 (2008).

2. M. J. Frisch, *et al* Gaussian 03, Revision D.02, Gaussian, Inc., Wallingford, CT, 2004.

3. D. S. Kilin and D. A. Micha, Chem. Phys. Lett. **461**, 266 (2008).

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