Computational studies of the optical properties of silicon compounds bonding to silver atoms and with group III and V substituents

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Systems composed of silicon chains and silicon rings, bonding to one or more Ag atoms, and containing substituents from group III (B and Al) or group V (N, P) have been computationally studied with density functional (DFT) and time-dependent DFT methods, to obtain their optical properties. Using codes in the Gaussian03 [1] package, calculations have provided atomic conformations, HOMO-LUMO excitation energies, electron binding energies, and electronic oscillator strengths. This allows calculation of rates of light absorption using equations from perturbation theory supplemented with information on line shapes [2]. Results are presented for the correlation between absorbed light wavelengths and rates versus the size and composition 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 the utilization of solar energy.

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

2. P. W. Atkins and R. S. Friedman "Molecular Quantum Mechanics", 3rd edition (Oxford Univ. Press, 1997), Chap. 12

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