Atomic basis size effects on the optical absorption intensities of silicon compounds bonding to silver atoms and with group III and V substituents

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Optical absorption intensities in the region of visible light, near IR and near UV spectra, have been calculated from excitation energies and oscillator strengths generated with the Gaussian03 package.[1] A study of numerous systems has been done to quantify the effect of atomic basis size on the values of the absorption intensities. 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. Calculations have provided atomic conformations, HOMO-LUMO excitation energies, electron binding energies, and electronic oscillator strengths, from which rates of light absorption have been obtained. [2] Results are presented for the correlation between absorbed light wavelengths and rates versus the size and composition of the systems. Analysis of the results provides insight on trends relevant to the absorption of sunlight.


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