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Optical Nonlinearity and Charge Transfer Analysis of Pyrene Adsorbed on Silver: Computational and Experimental Investigations

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Abstract

The interaction of pyrene on silver has been investigated using both experimental and computational methods. Hyperpolarizabilities computed theoretically together with experimental nonlinear absorption from open aperture Z-scan measurements, point towards a possible use of pyrene adsorbed on silver in the rational design of NLO devices. Presence of a red shift in both simulated and experimental UV-Vis spectra confirms the adsorption on silver, which is due to the electrostatic interaction between silver and pyrene, inducing variations in the structural parameters of pyrene. Fukui calculations along with MEP plot predict the electrophilic nature of the silver cluster in the presence of pyrene, with NBO analysis revealing that the adsorption causes charge redistribution from the first three rings of pyrene towards the fourth ring, from where the $2p$ orbitals of carbon interact with the valence $5s$ orbitals of the cluster. This is further confirmed by the downshifting of ring breathing modes in both the experimental and theoretical Raman spectra.

Keywords: Nonlinear Optics, electron density transfer, SERS, DFT, Adsorption, Fukui, Pyrene.

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