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A Time-Dependent Density Functional Theory Study of One-and Two-Photon Absorption: Stilbene- and Fluorene-Based Donor-Acceptor Chromophores RUTH PACHTER, PAUL DAY, KIET NGUYEN — In our ongoing theoretical studies to predict the photophysical properties of optical materials, we report the results for one-photon, and two-photon absorption (OPA and TPA) spectra, for a series of compounds, in which electron donating and accepting groups are attached to a core having a delocalized electron structure, such as stilbene or fluorene. Linear response time-dependent density functional theory, with hybrid exchange-correlation functionals, was applied in all calculations. We find that the calculated excitation energies are generally in good agreement with experiment, particularly when compared to measurements carried out in a nonpolar solvent. Predicted TPA cross-sections, applying the two-state approximation, are also in relatively good agreement with experiment; however, a lack of systematic experimental data on solvent effects limits a detailed comparison as yet.

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