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A Time-Dependent Density Functional Theory Study of One- and Two-Photon Absorption: Donor-Acceptor Chromophores. RUTH PACHTER, PAUL N. DAY, KIET A. NGUYEN, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio 45433-7702 — We report time-dependent density functional theory (TDDFT) calculations of one-photon, and two-photon absorption spectra, for a series of compounds, in which electron donating and accepting groups are attached to a core having a delocalized pi-electron structure, such as stilbene or fluorene. We find that the calculated excitation energies are in better agreement with experimental data upon the application of (x-c) functionals that take into account long-range interactions, and also by the inclusion of solvent effects. Furthermore, two-photon absorption cross-section predictions are improved with the application of quadratic response TDDFT, in comparison to experiment.

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