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Optical absorption in fluorenone-based push-pull molecules EDUARDO CRUZ-SILVA, PAUL J. HOMNICK, PAUL M. LAHTI, University of Massachusetts Amherst, VINCENT MEUNIER, Rensselaer Polytechnic Institute —
Push-pull organic molecules include both electron donor and acceptor substituents, which upon excitation induce a charge separation with potential uses in conductive polymers and light-harvesting materials for use in solar cells. In a recent work, a new set of such molecules using fluorenone as the electron-acceptor unit have been reported [1]. Here we present a comprehensive study of their electronic structure and and optical properties using time-dependent density functional theory (TDDFT) as implemented in the NWChem software suite [2]. The remarkable agreement between experimental and computed spectra among all test systems show that TDDFT can be readily used as a predictive tool for assessing and optimizing the optical properties on these systems. 1. P.J. Homnick and P.M. Lahti, Phys. Chem. Chem. Phys. 14, 11961-11968 (2012). 2. M. Valiev, E.J. Bylaska, N. Govind, K Kowalski, et al., Comput. Phys. Commun. 181, 1477 (2010).

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