

Abstract Submitted
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Ab Initio Generated UPS of Electron Donors¹ REESHMAH ALLEN, Center for Computational Material Science, Code 6392, Naval Research Lab, Washington, DC 20375, TUNNA BARUAH, Department of Physics, University of Texas at El Paso, El Paso Texas 79968, MARK R. PEDERSON, Center for Computational Material Science, Code 6392, Naval Research Lab, Washington, DC 20375 — We have calculated the ultraviolet photoelectron spectra (UPS) data for a variety of molecules that have been suggested for donors for organic photovoltaic materials. The method employed here uses NRLMOL and the PBE-GGA density-functional based method for approximating energies of molecules within a constrained occupation approach. The UPS data is then simulated by calculating the energy difference between the N-electron ground state and a large set of self-consistently generated (N-1)-electron states. Incorporating the relevant absorption probabilities is also discussed. Comparison of calculated UPS spectra to experiment allows us to determine the conditions under which self-interaction corrections¹ to the energy functional are necessary for determining accurate excitation energies will also be discussed. 1. M. R. Pederson, R. A. Heaton, and C.C. Lin J. Chem. Phys. 82, 2688 (1985).

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