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Effect of structural distortion and polarization in localization of electronic excitations in organic semiconductor materials IFFAT NAYYAR, Theoretical Div., Los Alamos National Lab, Los Alamos, NanoScience Technology Center and Dept. of Physics, University of Central Florida, Orlando, ENRIQUE BATISTA, Theoretical Div., Los Alamos National Lab, Los Alamos, SERGEI TRETIAK, Theoretical Div. and Center for Integrated Nanotechnoligies, Los Alamos National Lab, Los Alamos, AVADH SAXENA, DARRYL SMITH, RICHARD MARTIN, Theoretical Div., Los Alamos National Lab, Los Alamos — Organic polymers find varied applications in optoelectronic devices such as solar cells, light emitting diodes and lasers. Detailed understanding of charge carrier transport by polarons and excitonic energy transfer producing singlet and triplet excitations is critical to improve their efficiency. We benchmarked the ability of current functional models to describe the spatial extent of self-trapped neutral and charged excitations for MEH-PPV owing to its superior luminescence and experimental evidence. Now we are interested in distinguishing between two distinct origins leading to localization; spatial localization of the wavefunction by itself on the undistorted geometry and localization of the wavefunction assured by distortion of the structure during its relaxation. We suggest localization is produced by electronic rearrangements and character of the functional. We also observe that different functionals place the highest occupied and lowest virtual orbitals at different positions in the energy band diagram based on their ability to predict the extent of localization of these states.

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