

Abstract Submitted  
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**Effect of environment and long range behaviour of exchange functional on polaron formation in  $\pi$ -conjugated polymers** IFFAT NAYYAR, Theoretical Div, Los Alamos National Lab, NM and NanoScience Technology Center, Dept. of Physics, University of Central Florida, Orlando, FL, ENRIQUE BATISTA, SERGEI TRETIAK, AVADH SAXENA, DARRYL SMITH, RICHARD MARTIN, Theoretical Division, Los Alamos National Lab, NM — Organic conjugated polymers find a variety of applications in devices such as solar cells, light emitting diodes and lasers. An accurate understanding of the role of nonlinear excitations as polarons in charge carrier transport is critical to improve the efficiency of these devices. PPV and MEH-PPV are the candidates of choice for the extensive experimental data and relative simplicity compared to other polymers. This motivated us to perform a density functional theory study to describe the charge defects in these systems. We emphasize on the role of surrounding dielectric medium and the amount of long range orbital exchange in the density functional to predict the polaron localization in agreement with experiment. The particle-hole symmetry observed in trans-geometries is broken by introducing certain cis defects.

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