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Influence of *trans* and *cis* defects on the localization of charged excitations in π -conjugated organic polymers IFFAT NAYYAR, Theoretical Div., Los Alamos National Laboratory, NM, NanoScience Technology Center and Dept. of Physics, University of Central Florida, Orlando, FL, ENRIQUE BATISTA, Theoretical Div., Los Alamos National Laboratory, NM, SERGEI TRETIAK, Theoretical Div. and Center for Integrated NanoTechnologies, Los Alamos National Laboratory, NM, AVADH SAXENA, DARRYL SMITH, RICHARD MARTIN, Theoretical Div., Los Alamos National Laboratory, NM — Optoelectronic devices with π -conjugated polymers are in demand for use in light-emitting diodes (LED), solar cells and lasers. A recent study predicted differences in the response of the hyperfine field by polaronic species in organic LEDs. The improved fluorescence exhibited by different isomeric forms of PPV derivatives in these devices motivated us to investigate the influence of various conformational defects of *trans* and *cis* nature on the energetics and localization of positive (P^+) and negative (P^-) polarons using density functional theory. We observe the P^+ and P^- states are highly sensitive on the structural conformation and atomic charge distributions. The P^- state is observed to be more localized than P^+ in consistent with recent experiments when the polarization effects are included. These defects not only break the particle-hole symmetry but demonstrate higher charge-carrier mobilities for holes than electrons. This helps in tuning the charge-transport and photo-physical properties of organic materials by understanding their structure-property correlations for technological innovations.

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