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Charge and energy transports via poly-phenylacetylene based dendrimers YONGWOO SHIN, MINGHAI LI, XI LIN, Boston University — Poly-Phenylacetylene (PPA) is widely used in photoconductivity, photoluminescence, and light harvesting applications. In this work, we investigate the charge and exciton transport energetics and mechanisms in the PPA-based dendrimers using our recently developed adapted Su-Schrieffer-Heeger (SSH) model Hamiltonians and *ab initio* Hartree-Fock (HF) calculations. We found both doping and photo-excitation lead to the formation of optical phonon dressed pi electron states, namely the self-localized polarons, in the energy gap. Independent from their origins, these polarons can be self-trapped at multiple lattice locations along the PPA chain, and migrate from one to the next with an activation barrier of $\sim$0.006 eV, slightly higher than the corresponding barrier found in *trans*-polyacetylene. The PPA-based dendrimers can be constructed via the meta-positions of phenyl rings. In this case, we found the dendrimer junctions form attractive potential wells for both polarons and excitons, and the width and height of these junction potential wells can be controlled by the geometry of the dendrimers.

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