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Mobility of self-localized defects in conjugated dendrimers YONGWOO SHIN, XI LIN, Boston University — In our previous study we have computed the intrinsic activation barrier for a topological soliton moving along a linear trans-polyacetylene chain. In this work we systematically investigate the adiabatic potential energy surfaces of self-localized defects, such as soliton, polaron, bipolaron, and exciton, at the dendrimer triple junctions using the Su-Schrieffer-Heeger (SSH) model Hamiltonian and ab initio calculations. All junction structures are found to be attractive energy basins for these self-localized defects. In particular, excitons can be trapped by a pair of closely positioned triple junctions with the hole and electron states both displaying separated charge density distributions. Under an external electric field, excitons can be split into spatially separated electrons and holes, localized at different junctions on the conjugated dendrimer.

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