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A molecular heterojunction of zinc phthalocyanine and peanut-shaped fullerene polymer: A density functional study

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Abstract

We have performed first-principles density functional calculations of a molecular heterojunction of a zinc phthalocyanine (ZnPc) molecule and a peanut-shaped fullerene polymer (PSFP) made from several coalesced cross-linked C₆₀ molecules. The PSFP has many isomers and all have both spatially localized (near ZnPc) and metallic conducting levels. Here we consider four typical isomers. From the resulting electronic structure, we discuss the applicability of these isomers to organic photovoltaics (OPV), electrodes, and light harvesting materials. If one of the isomers called T3, which has the largest energy gap, is used together with ZnPc for OPV, this system shows more than 20 % energy conversion efficiency.

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