THREE-DIMENSIONAL POLYMER-FULLERENE HETEROJUNCTION

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ABSTRACT

Researches on the electronic characteristics of the fullerene have proven its importance to build efficient solar cells. Polymer-fullerene based junctions, such as the PCBM, have resulted in flexible and highly efficient solar cells. Thus, we present a study of the electronic behavior of a fullerene (C60) molecule attached to six orthogonal polymer junctions (phenylpropanodinilla (PPP) and tetrathiafulvalene (TTF)) that works as a three-dimension rectifier. In order to understand the electronic transport in the molecule, we applied non-equilibrium green function (NEGF) method and performed Fowler-Nordheim (FN) and Millikan-Lauritsen (ML) analyses. We confirmed that the fullerene works not only as an electron donor, but also as barrier and transport channel to electrons through the molecule, and the ML curves proved to be sufficient to describe the FN characteristics. Moreover, when the phenyl groups are orthogonally subjected to bias voltage, the charge distribution and the current displays regions of saturation and resonance similar to semiconductor devices. Therefore, in this work, we report the theoretical design of a three-dimensional photoactive device.

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