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THEORETICAL CHARACTERIZATION OF THE ORGANIC SOLAR CELL (PC60BM:P3HT) FOR SPACE ENVIRONMENT CONDITIONS

Abstract

Nowadays the technology that has attracted the attention of many companies, academies and research centres is on the organic photovoltaic (OPV) for solar cells. The development of materials used in these cells has had a rapid interest since the discovery of its potential use, because they combine common plastics properties, however, they are flexible, non-polluting and of low weight. Also, exist a lot of papers about its function but just in the earth but its necessary to know space environment effects on the key parameters of the OPV cells, id est, characterization under space environment conditions. We use time-dependent density functional theory together with a set of extensive multidimensional visualization techniques to characterize band gap, optical absorption properties, intramolecular and intermolecular charge transfer, exciton binding energy, charge transfer integral, and the rate of charge transfer and recombination in the $PC_{60}BM$:P3HT model of an organic solar cell. These theoretical methods and calculation techniques not only promote deeper understanding of the connection between chemical structures and the optical and electronic properties of the donor-acceptor system in the space environment but also can be used to rational design novel donor-acceptor system specifically for space conditions.