

Theoretical study of aromatic-antiaromatic pairs as material in organic solar cells of double light harvesting

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Molecular light harvesting components of organic solar cells containing antiaromatic and aromatic molecules as organic semiconductors were studied. We found that antiaromatic molecules with indacene core can act as acceptors looking for new options to assemble donor/acceptor interfaces. This is supported by their properties such as molecular orbitals energies, rigid fused core that could promote π - π intermolecular interactions imparting ordered nanostructures, that let high charge mobility thanks to their properly low reorganization energy and the optimum energy offsets of the donor/acceptor interfaces. It was found that pentacene might be an excellent donor and the benzo[g]benz[6,7]indeno[1,2-b]fluorene could act as an acceptor. © 2016 Elsevier B.V.

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Indacene

Organic solar cells

Reorganization energy

Aromatic compounds

Molecular orbitals

Molecules

Nanostructured materials

Semiconducting organic compounds

Solar cells

Antiaromatic molecules

Aromatic molecules

Donor/acceptor interface

Indacene

Indeno[1,2-b]fluorene

Intermolecular interactions

Ordered nanostructures

Reorganization energies

Organic solar cells