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Iván Martínez, Eduardo Schott, Ivonne Chávez, Juan Manuel Manríquez, Ximena Zarate

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

Iván Martínez,^{*b} Eduardo Schott,^a Ivonne Chávez,^a Juan Manuel Manríquez,^{a,b} Ximena Zarate^{*c}

^aDepartamento de Química Inorgánica, Facultad de Química, Pontificia Universidad Católica de Chile. Avda. Vicuña Mackenna 4860, Santiago, Chile.

^bLaboratorio de Bionanotecnología, Universidad Bernardo O'Higgins, General Gana 1780, Santiago, Chile.

^cInstituto de Ciencias Químicas Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile. Av. Pedro de Valdivia 641, Santiago, Chile.

Abstract

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.

Keywords: Organic solar cells; DFT; indacene, reorganization energy.

1. Introduction

In the last decades, there has been an enormous effort to develop high efficient organic solar cells (OSCs). These cells are mainly composed of a donor and an acceptor material where the

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