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Packing and Disorder in Substituted Fullerenes

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JOURNAL OF PHYSICAL CHEMISTRY C Volume: 120 Issue: 31 Pages: 17242-17250

DOI: 10.1021/acs.jpcc.6b05197 Published: AUG 11 2016 **View Journal Impact**

Abstract

Fullerenes are ubiquitous as electron-acceptor and electron-transport materials in organic solar cells. Recent synthetic strategies to improve the solubility and electronic characteristics of these molecules have translated into a tremendous increase in the variety of derivatives employed in these applications. Here, we use molecular dynamics (MD) simulations to examine the impact of going from monoadducts to bis- and tris-adducts on the structural, cohesive, and packing characteristics of [6,6]-phenyl-C-60butyric acid methyl ester (PCBM) and indene-C-60. The packing configurations obtained at the MD level then serve as input for density functional theory calculations that examine the solid-state energetic disorder (distribution of site energies) as a function of chemical substitution. The variations in structural and site-energy disorders reflect the fundamental materials differences among the derivatives and impact the performance of these materials in thin-film electronic devices.

Keywords

KeyWords Plus: ORGANIC SOLAR-CELLS; ACID METHYL-ESTER; ELECTRON-TRANSPORT; CHARGE-TRANSPORT; PHOTOVOLTAIC PERFORMANCE; SOLUBILIZING GROUPS; ENERGETIC DISORDER; PC71BM FULLERENES; PCBM; FIELD

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Funding

Funding Agency	Grant Number
Deanship of Scientific Research of King Abdulaziz University	D-001-433
Department of the Navy - Office of Naval Research under the MURI "Center for Advanced Organic Photovoltaics"	N00014-14-1- 0580 N00014-16-1- 2520
King Abdullah University of Science and Technology	
KAUST	
Office of Naval Research - Global	N62909-15-1- 2003
University of Kentucky Vice President for Research	

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Publisher

AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA

Categories / Classification

Research Areas: Chemistry; Science & Technology - Other Topics; Materials Science

Web of Science Categories: Chemistry, Physical; Nanoscience & Nanotechnology; Materials Science,

Multidisciplinary

Document Information

Document Type: Article
Language: English

Accession Number: WOS:000381452000011

ISSN: 1932-7447

Other Information IDS Number: DT4LG

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