Packing and Disorder in Substituted Fullerenes

By: Tummala, NR (Tummala, Naga Rajesh)[1,2]; Elroby, SA (Elroby, Shaaban A.)[3,4]; Aziz, SG (Aziz, Saadullah G.)[3]; Risko, C (Risko, Chad)[5,6]; Coropceanu, V (Coropceanu, Veaceslav)[1,2]; Bredas, JL (Bredas, Jean-Luc)[1,2,7]

View ResearcherID and ORCID

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-60-butyric 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

Author Information

Reprint Address: Tummala, NR; Bredas, JL (reprint author)

+ Georgia Inst Technol, Sch Chem & Biochem, Atlanta, GA 30332 USA.

Reprint Address: Tummala, NR; Bredas, JL (reprint author)

+ Georgia Inst Technol, Ctr Organ Photon & Elect, Atlanta, GA 30332 USA.

Reprint Address: Bredas, JL (reprint author)

+ King Abdullah Univ Sci & Technol, Phys Sci & Engn Div, Solar & Photovolta Engn Res Ctr, Thuwal 239556900, Saudi Arabia.

Addresses:

+ [1] Georgia Inst Technol, Sch Chem & Biochem, Atlanta, GA 30332 USA

+ [2] Georgia Inst Technol, Ctr Organ Photon & Elect, Atlanta, GA 30332 USA

− [3] King Abdulaziz Univ, Dept Chem, Jeddah 21589, Saudi Arabia
Organization-Enhanced Name(s)
King Abdulaziz University

+ [4] Beni Suef Univ, Dept Chem, Fac Sci, Bani Suwayf 62511, Egypt

+ [5] Univ Kentucky, Dept Chem, Lexington, KY 40506 USA

[6] Univ Kentucky, Ctr Appl Energy Res CAER, Lexington, KY 40506 USA

[7] King Abdullah Univ Sci & Technol, Phys Sci & Engn Div, Solar & Photovolta Engn Res Ctr, Thuwal 239556900, Saudi Arabia

E-mail Addresses: nagarajesh@gatech.edu; jean-luc.bredas@kaust.edu.sa

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	

View funding text

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

Cited References in Web of Science Core Collection: 59

Times Cited in Web of Science Core Collection: 3