Thermal Narrowing of the Electronic Bandwidths in Organic Molecular Semiconductors: Impact of the Crystal Thermal Expansion

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JOURNAL OF PHYSICAL CHEMISTRY LETTERS

Volume: 3 Issue: 22 Pages: 3325-3329

DOI: 10.1021/jz301575u

Published: NOV 15 2012

View Journal Impact

Abstract

We report on electronic-structure calculations for the pentacene and rubrene crystals, based on experimental crystal geometries measured at different temperatures. The results are in very good agreement with angle-resolved photoelectron spectroscopy data that indicate that the widths of the valence and conduction bands in both materials become narrower at higher temperatures. Our findings strongly suggest that the thermal bandwidth narrowing in the pentacene and rubrene crystals is primarily caused by the thermal expansion of the lattice rather than by a renormalization of the transfer integrals induced by a polaron effect. The effect of thermal expansion on the charge-transport properties is also discussed.

Keywords

KeyWords Plus: CHARGE-TRANSPORT; SINGLE-CRYSTALS; NAPHTHALENE; PENTACENE; MOTION

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Funding

Funding Agency	Grant Number
National Science Foundation under the STC Program	DMR-0120967
MRSEC Program	DMR-0819885
CRIF Program	CHE-0946869

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; Physics

Web of Science Categories: Chemistry, Physical; Nanoscience & Nanotechnology; Materials Science, Multidisciplinary; Physics, Atomic, Molecular & Chemical

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000313770400015

ISSN: 1948-7185

Other Information

IDS Number: 073VE

Cited References in Web of Science Core Collection: 35

Times Cited in Web of Science Core Collection: 28