Article

Charge Transfer in Molecular Complexes with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F_4-TCNQ): A Density Functional Theory Study

Lingyun Zhu, Eung-Gun Kim*, Yuanping Yi, and Jean-Luc Brédas*
School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, United States

Chem. Mater., **2011**, *23* (23), pp 5149-5159
DOI: 10.1021/cm201798x
Publication Date (Web): November 8, 2011

E-mail: eg.kim@dankook.ac.kr; jean-luc.bredas@chemistry.gatech.edu.

Abstract Supporting Info
Full Text HTML Figures
Hi-Res PDF [3528 KB]
PDF w/ Links [570 KB]

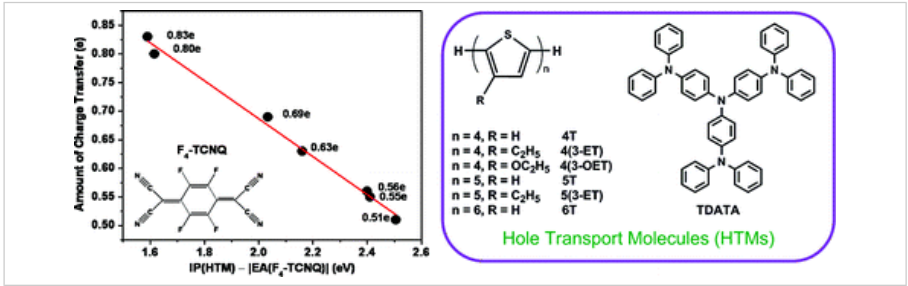
†**Author Present Address**
Department of Polymer Science and Engineering, Dankook University, Jukjeon, Gyeonggi 448−701, Korea.

‡**Author Present Address**
Department of Chemistry, King Abdulaziz University, Jeddah 21589, Saudi Arabia.

Note
There was an error in section 3.4 in the version published ASAP November 8, 2011; the corrected version published ASAP November 10, 2011.

Section: Physical Organic Chemistry

Abstract



Molecular doping is a charge-transfer process intended to improve the electrical properties of organic semiconductors and the efficiency of organic electronic devices, by incorporation of a complex-forming, strong molecular electron acceptor or donor. Using density functional theory methods with dispersion corrections, we seek to monitor charge transfer and estimate its amount via calculations of experimental observables. With 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F_4-TCNQ) as a *p*-dopant (electron acceptor) and an array of π-conjugated molecules as hole-transport materials (donors), the amount of charge transfer is seen to be a non-monotonic function of the offset defined by the donor ionization potential

History
Published In Issue
December 13, 2011
Article ASAP
November 08, 2011
Received: June 23, 2011
Revised: October 17, 2011

(IP) and the acceptor electron affinity (EA), IP − |EA|. Interestingly, a well-defined, *linear* relationship between the amount of charge transfer and IP − |EA| is obtained when the IP and EA values are adjusted to reflect intramolecular geometric changes in the final form of the complex. This study offers a straightforward way to match donor–acceptor pairs with desired doping effects and to estimate the resulting charge density in organic semiconductors.

Keywords: molecular doping; charge transfer; molecular complexes; organic semiconductors; IP−EA offset; DFT