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### Charge Transfer in Molecular Complexes with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F<sub>4</sub>-TCNQ): A Density Functional Theory Study

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Abstract

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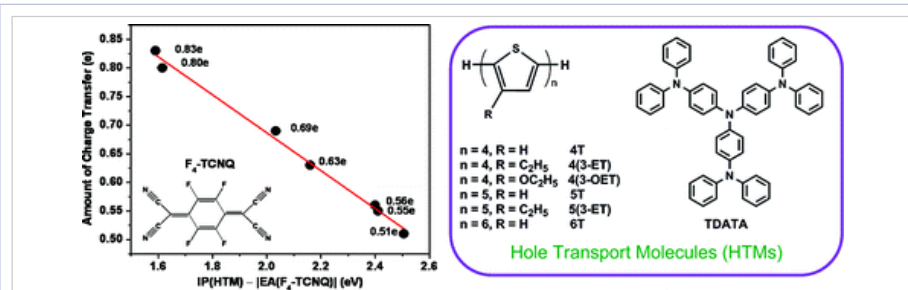
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#### Note

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<sub>4</sub>-TCNQ) as a *p*-dopant (electron acceptor) and an array of  $\pi$ -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

(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



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