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Emerging Technologies with Advanced Devices from Micro to Nano

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Modelling of n-type Materials Based on [D-π-A] Structure for the Application in Organic Field Effect Transistors: DFT Study

Ankit Kargeti, Tabish Rasheed, and Shamoon Ahmad Siddiqui

Abstract OFETs (Organic Field Effect Transistors) are widely researched since the first reported OFET in 1986 which was made of Polythiophene. We designed two novel molecular structures based on Donor-pi-Acceptor or [D-π-A] model to look upon their efficient use in Organic field effect transistors. The designed systems are named as system first S1 (anthracene-pyrrole-butanoic acid), and system second S2 (naphthalene-pyrrole-butanoic acid). Both the structures were optimized under the framework of density functional theory with B3LYP/6–31 + G(d, p) basis set on a Gaussian16W software package. The calculated parameters are hole's reorganization energy λ_h, electron's reorganization energy λ_e, HOMO–LUMO energy gap, dipole moment. Further, we have looked upon their electric field dependence of the HOMO–LUMO energy gap and dipole moment for all the molecules. Both the designed molecules S1 and S2, are found to be suitable for designing as n-type semiconducting channel for OFETs.

Keywords OFET · D-π-A · n-Type and p-Type semiconductors · DFT · HOMO–LUMO gap energy · Reorganization energy of holes and electrons

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