Insight into the semiconducting performance of tetraphenyldipyranylidene derivatives in organic field-effect transistors

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Abstract

In this paper, Tetraphenyldipyranylidene (DPPh), a large quinoidal planar π-conjugated heterocyclic, was considered as primary organic molecule in organic field effect transistors (OFETs). Electron-withdrawing atoms such as F, Cl, and Br were attached to the H-atoms of four peripheral phenyl groups of para-positions relative to the O-atoms of DPPh. Density functional theory (DFT) calculations at the M06-2X/6-311G++ (d,p) level were performed. The influences of the different electron-withdrawing atoms such as F, Cl, and Br on the electronic and optical properties, charge transport parameters, and charge carrier mobility were investigated. The absorption and emission spectra of the DPPh and its derivatives were theoretically simulated in OFETs. The simulated spectra show an intense peak in the visible region (400-650 nm), in which the highest adsorption/emission intensity is related to DPPh-Br. Moreover, the charge injection energy barrier of DPPh and its derivatives were calculated by considering Pt as the source electrode. Based on the results, a greater hole transport is predicted than the electron transport. Moreover, the obtained ratio of the hole/electron mobility and the theoretical correlations between the charge transport parameters of monomers and dimers show that the insertion of the electron-withdrawing atoms in the DPPh structure is a promising strategy to have an ambipolar or n-type semiconductor, too. The obtained results show that introducing electron-withdrawing atoms at the para-position of the DPPh improves the hole/electron injection and transport process in the OFET devices. Finally, DPPh-Br shows a great performance in comparison with the substituted F and Cl atoms in the OFETs devices.

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