The Effect of Constitutional and Conformational Isomerization on the Electrical Properties of Diblock Molecular Diode

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Abstract:

The ultimate goal of this paper is to introduce new links between the chemical response of the molecule to the electric field and the physics of cell involving the molecule. Density functional theory (DFT) calculations were performed to investigate the effect of constitutional and conformational isomerization on the electrical properties of the dipyrimidinyl-diphenyl dithiol (DPDPh1) as a diblock molecular diode. The non-equilibrium Green’s function approach combined with DFT (NEGF-DFT) has been used to compute the current–voltage characteristics in order to support the obtained results. The calculations could differentiate among the isomers regarding their rectification efficiency. Moreover, plots of the global electrophilicity index and the tendency of constitutional isomers to receive charge from the circuit against applied voltage show I–V curve feature. The conformational analysis has been done through examining the effect of structural twist on the current, dipole moment, HOMO energy, and molecular gain of the DPDPh1 molecule. The rectification is slightly affected by twisting because of the limited change in molecular polarization. However, the results demonstrated that the insertion of a CH2-spacer or twisting the donor and acceptor parts of the DPDPh1 molecule by 90° generates an Aviram–Ratner-like diode where the HOMO and LUMO are localized on the donor and acceptor subunits, respectively.

Keywords:

Molecular diode; Constitutional and conformational isomery; DFT; NEFG; Electric field; Current–voltage curve

Published In:

Organic Electronics, 12, 1080-1092