Modification of the Electric Properties of Molecular Devices via Gradual Increment of Number of Nitrogen Atoms

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Abstract:

This paper introduces a new means to manipulate electronic structures and, consequently, the electrical properties of molecular devices via gradual increase of number of nitrogen atoms in the backbone of conjugated organic molecular systems. Diblock molecules were selected for this purpose. Density functional theory (DFT) was used to investigate geometrical and electronic structures in the absence and presence of external electric field. Furthermore, the tendency of the anchor sulfur atoms toward electrodes in a simulated closed circuit was estimated from the relative condensed Fukui function. The obtained results indicated that HOMO–LUMO gap decreases steadily with increasing the number of nitrogen atoms, which would be used as a means for modifying the electrical properties in a regular mode.

Published In:

Organic Electronics, 13, 807-814