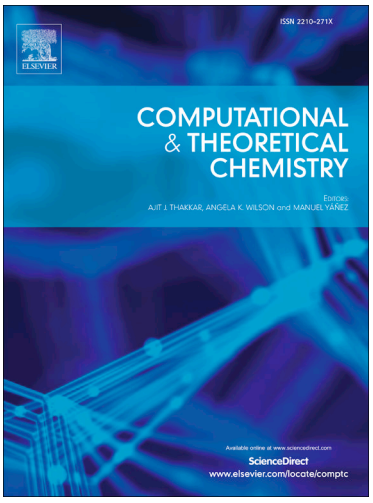

Charge Injection and Hopping Transport in bridged-dithiophene-Triazole-bridged-dithiophene (DT-Tr-DT) Conducting Oligomers: A DFT Approach

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Charge Injection and Hopping Transport in bridged-dithiophene-Triazole-bridged-dithiophene (DT-Tr-DT) Conducting Oligomers: A DFT Approach

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Abstract

Here, we have reported a series of exciting conducting organic heterocyclic oligomers possessing the cyclopentadithiophene-4-thione-triazole-cyclopentadithiophene-4-thione (DT-Tr-DT) as basic unit based on the donor-acceptor (D-A) approach. The basic unit is substituted with different electron-withdrawing and donating groups to tune its structural and electronic properties. Density functional theory (DFT) and time-dependent DFT methodologies were utilized to investigate the ground and excited state calculation. Here, our main focus is on the HOMO-LUMO gaps, electronic transition, charge transfer rate and the reorganization energies (λ). Our study reveals that the designed oligomers under investigation exhibit excellent charge transfer rates. Furthermore, it has also been reported that oligomers substituted with the electron-donating groups exhibit lower Δ_{H-L} values compared to the electron-withdrawing groups. Therefore, oligomers substituted with electron-donating moieties will become potential candidates for fabrication of organic light emitting diodes (OLEDs), organic field effect transistors (OFETs), photovoltaic cells and solar cells.

Keywords: Optoelectronic properties, Triazole, DFT, TDDFT, Reorganization energy, Hole transfer rates

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