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Theoretical Study of Charge Transport in Alternating Donor-Acceptor Complex Oligomers for Polymer Solar Cell Applications: Poly(3-hexylthiophene) Based Azole

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In this research have been simulated geometrical structures, molecular orbital, charge transports and photophysics of complex alternating donor-acceptor oligomers using in photo-active layer of polymer solar cell applications. Poly(3-hexylthiophene) (P3HT) was selected as an electron donor, while different azole such as oxadiazole (OXD), triazole (TAZ) and thienothiadiazole (TD) were used as electron acceptors, resulting in donor-acceptor complex oligomers P3HT-OXD, P3HT-TAZ and P3HT-TD, respectively. The calculation was performed by using Gaussian 09W software package at density functional theory (DFT) level with B3LYP (Becke Three-parameters Lee–Yang–Parr) exchange correlation functional and 6-31G(d) basis sets. Simulation results obtained that energy levels HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) from all isolated electron acceptor molecules (OXD, TAZ and TD) are lower than that of the isolated electron donor (P3HT) indicating that all acceptors can withdraw electrons from the donor molecule. However, analyzing geometrical structure results were revealed that P3HT-OXD and P3HT-TD monomers reveal planarized structure, while TAZ unit from P3HT-TAZ molecule shows twisted conformer. Analyzing of molecular orbitals from complex oligomers were found that at LUMO level, electron transported from the donor to the acceptor unit was found from all complex oligomers but less for P3HT-TAZ due to large torsional angle between donor and acceptor units. Intramolecular charge transfer can be verified by Mulliken population analysis (Mulliken charge) on the acceptor unit. We obtained that OXD provides strongest electron withdrawing than others and polymer of P3HT-OXD can absorb wavelength of light well at 420 nm which is closed to maximum intensity range (around 550 nm) from solar spectrum compared to other (P3HT-TAZ = 371 nm, P3HT-TD = 3024 nm), indicating that OXD behaves as a good electron acceptor. We concluded that OXD provides appropriate characteristics of an electron acceptor unit for complex donor-acceptor using for polymer solar cell application.

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