Pervin Unal Civcir, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

A Theoretical Calculations of Band Gaps of conducting polymers with electron donor–acceptor unit

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The interaction between alternating donors and acceptors results in a diminished band gap. With determining the proper donor (D) and acceptor (A) groups, it is possible to decrease the band gap (<1.8 eV) as much as possible or to adjust HOMO (highest occupied molecular orbital)-LUMO (lowest unoccupied molecular orbital) levels. Therefore, in this study the theoretical methods were used for the modelling of the donor–acceptor type conjugated polymers. Quantum chemical calculations were performed using density functional theory (DFT) to investigate the HOMO–LUMO energy gap of benzothiadiazole based donor–acceptor type conjugated polymers: poly{4,7-bis(3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)benzo[c][1,2,5]thiadiazole} (P1), poly{4,7-bis(3,3-dimethyl-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)benzo[c][1,2,5]thiadiazole} (P2), poly{4,7-bis(3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)-5,6-diphenylbenzo [c][1,2,5]thiadiazole} (P3) and poly{4,7-bis(3,3-dimethyl-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)-5,6-diphenyl-benzo[c][1,2,5] thiadiazole} (P4). DFT is one of the most successful quantum chemistry tools for the description of ground-state properties of metals, semiconductors and insulators. Compared to other quantum chemistry methods, the DFT approach gives low computational cost and accurate results. The geometries of the monomers and oligomers were optimized using semi-empirical PM6 method in the gas phase. The band gaps of the polymers were performed by the B3LYP level of theory (Becke three-parameter hybrid correlation functional combined with Lee–Yang–Parr correlation functional) with 6-31G(d) basis set. Band gaps of the studied polymers were obtained by extrapolating oligomers gaps to infinite chain lengths. The results indicate that calculated band gaps are in good agreement with the experimental values in the literature. The theoretical methods used in this study are promising for the modelling of similar donor–acceptor type novel conjugated polymers.

Biography

Civcir completed her PhD at the University of East Anglia, UK in 1992 and became a professor in Ankara University in 2009. She is a lecturer in Ankara University, Faculty of Science, Chemistry Department. She works in the field of Organic and Computational Chemistry and has published more than15 papers in reputed journal. She has written a Chemistry book in Turkish. She was involved in translating the five Chemistry books from English to Turkish.

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