Nevin Kaniskan, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-008

DFT studies on copolymers of 3,4-Ethylenedioxythiophene/3-methylthiophene and pyrene

Nevin Kaniskan
Anadolu University, Turkey

Conducting polymers, superior electrical, electronic, magnetic, and optical properties of compounds are very important in the industry. They are named as the "synthetic metal" or "organic metal". Thiophene can be prepared easily and have high conductivity. Therefore, too much theoretical work has been done until now. However, it is very little theoretical work about derivatives of these compounds. Since the interaction between alternating donors and acceptors results in a diminished band gap, a low band gap (<1.8 eV) will be expected in polymers containing donor–acceptor (D–A) repeating units. In order to predict the band gaps for guiding the synthesis of novel materials with low band gaps, we apply quantum-chemical techniques to calculate the band gaps in several polythiophene homo- and copolymers: poly{3-methylthiophene} (P1), poly{2,3-dihydrothieno[3,4-b][1,4]dioxine}, EDOT (P2) and polypyren (P3), poly{5-(4-methylthiophen-2-yl)-2,3-dihydrothieno[3,4-b][1,4]dioxine} (P3), poly{3-methyl-2-(pyren-1-yl) thiophene} (P4), and poly{5-(4-methyl-5-(pyren-1-yl)thiophen-2-yl)-2,3-dihydrothieno[3,4-b][1,4]dioxine} (P5). The geometries of the oligomers were optimized using semi-empirical PM6 method. The band gap calculations on these oligomers were performed by density functional theory (DFT) (B3LYP/6–31G(d,p). Band gaps of the corresponding 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 addition, depending on the type of substituent and the substitution pattern, large differences in the delocalization pattern are observed between the substituted and unsubstituted oligomers. It is found that the band gaps critically depend on the chemical structures.

Biography

Nevin Kaniskan has completed her PhD in 1989 from Anadolu University. She is associated proffessor of Anadolu University at Chemistry Department.

nkaniska@anadolu.edu.tr

Notes: