Design of Thiophene and Thiadiazoloquinoxaline Containing Semiconducting Polymer

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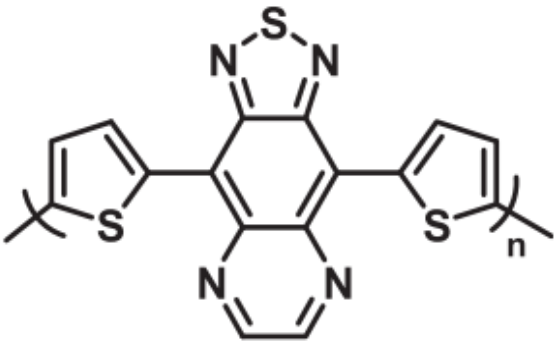
Quinoxaline is a compound known as aromatic heterocyclic that has a benzene ring joined to a pyrazine group [1]. Quinoxaline itself is of scientific interest, and the quinoxaline derivatives are used in pharmaceuticals, dyes and antibiotics. Also, polymers containing quinoxaline have lower band gaps. Quinoxaline is used as electron acceptor unit (A) in semiconducting polymer systems. In this study, donor-acceptor-donor (D-A-D) type conjugated polymer based on quinoxaline acceptor was designed and electronic properties were calculated. The most stable structures of the monomer and oligomers, consisting of thiophene (D) and thiadiazoloquinoxaline (A) groups were determined. HOMO-LUMO energies of the structures were obtained by using B3LYP/6-31G (d) and B3LYP/LANL2DZ calculations without and with the inclusion of the PCM. Electronic band gap (Eg) values of all structures were obtained from the difference of HOMO and LUMO energies. Eg value of the polymer was found by extrapolation and linear fitting methodology. The results obtained from different calculation levels were compared with the experimental results.



[1] S. Achelle, C. Baudequin, N. Plé, *Dyes and Pigments*, **2013**, 98, 575-600

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