The Impact of the Conjugation Pathway in Benzobisaxozole-Containing Polymers from Theory & Experiment

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Recent developments in the synthesis of functional benzobisoxazoles have led to new benzobisoxazole-containing polymers that possess two possible conjugation pathways. One such pathway is through the oxazole rings (pathway A) while the second is directly through the central benzene ring (pathway B), leaving the oxazole rings perpendicular to the polymer backbone. In order to probe the structure-property relationships that exist between these different configurations, three polymers featuring each conjugation pathway were synthesized by our collaborators. We performed density functional theory (DFT) and time-dependent density functional theory B3LYP/SVP treatments on set of oligomers possessing these morphologies. Long chain limit computations were performed in order to model the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) and band gaps for each set of polymers. All computations were generated using Gaussian09 on San Diego Supercomputing Center's Gordon Cluster through National Science Foundations Extreme Science and Engineering Discovery Environment.