ABSTRACT

Sustainable and cost-efficient energy equipment has become a significant aspect, as a result of the exhaustion of fossil fuels and increase in energy consumption. The potential of organic solar cells (OSCSs) is great due to their light, tunable and flexible electronic properties. Two molecules BTD-IC and QTP-IC were constructed in this study to study the D-A systems using Thiophene and benzothiadiazole (BT). The DFT and TD-DFT methods were used to study the designed molecules BTD-IC and QTP-IC in order to know about their optimized geometrical, electronic behavior and optoelectronic characteristics. The various properties that were assessed include the HOMO-LUMO energy levels and their band gaps, normalized absorbance spectra in the gas phase, photo physical properties, molecular solubility factor, chemical descriptors analysis They have been used to assess their photovoltaic potential in terms of parameters such as HOMO-LUMO, and electron-hole transition analysis (TDM). The synthesized BTD-IC molecule exhibits efficient transfer of charge-carriers and band gaps of energy level that are encouraging towards conversion of solar energy. In my synthesis work, **BTD-IC** were synthesized and its characterization was done by performing different techniques like UV-Vis, FTIR, GC-MS and NMR spectroscopy. Overall, BT-thiophene conjugated systems, particularly **BTD-IC** demonstrate strong potential for energy conversion technologies and next-generation OSCs. In my synthesis work, **BTD-IC** were synthesized and its characterization was done by performing different techniques like UV-Vis, FTIR, GC-MS and NMR spectroscopy. Hence, BT-thiophene conjugated systems, particularly **BTD-IC** demonstrate strong potential for energy conversion technologies and next-generation OSCs.