

Abstract Submitted
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A Quantum Chemical Study of Structural and Electronic Properties of DTBT and DTBT:C70 Complexes¹ MESFIN TSIGE, RAM BHATTA, Department of Polymer Science, The University of Akron — Organic photovoltaic (OPV) devices containing the dithienyl-benzothiadiazole (DTBT) based conjugated polymers are promising candidates for solar energy harvesting. Practical realization of OPV devices requires further improving their performance, which relies on the fundamental understanding of the morphology and electronic properties of DTBT-based polymers. Nevertheless, even the conformational properties of DTBT have not been fully revealed yet. Here, we present the quantum chemical calculations of the structural and electronic properties of DTBT as well as DTBT:C70 complexes at the molecular level. These first principles results include the two-dimensional potential energy surface, the band gap, DTBT:C70 equilibrium distance as well as the energy level offset at the interface compared to the energy levels of the individual material. The computed results are compared to the available experimental data.

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