A TIME DEPENDENT DENSITY FUNCTIONAL STUDY OF BENSOBISAZOLES

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The demand for energy efficient and environmentally friendly alternatives to fossil fuel is on the rise. A particular area of interest involves conjugated polymers whose distinct properties (mechanical flexibility, light weight, low cost of mass production) make them appealing to the solar and fuel cell industries. In this study, time dependent density functional theory (TDDFT) is applied to an array of tunable materials comprised of benzobisazoles. The HOMO, LUMO and band gaps of the most promising structures will be discussed.