The Impact of Push/Pull Ring Systems locations in Benzobisaxozole Possessing Cruciforms

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Asymmetric donor-acceptor benzobisoxazole dyes are systems of interest for electronic devices and in imagining and probing applications due to their ease of synthesis and optical properties. The donor and acceptor groups bonded off of the core create a large dipole, which can result in an intramolecular charge transfer in the excited state, producing a low band gap and emission in near-infrared. This study focuses on the effect of the donor/acceptor system's locations off of the benzobisaxozole core in either the perpendicular of the parallel axis. Two thiol rings were placed off the core in the opposite axis of the push/pull system, resulting in the cruciform structure. Here we will provide density functional theory (DFT) and time-dependent density functional theory (TD-DFT) computations on a set of push-pull systems using B3LYP/6-31G*. The HOMO, LUMO, and optical band gaps were generated and compared. In addition, the electrostatic potential maps and the frontier orbitals were examined. All computations were generated using Gaussian09 on San Diego Supercomputing Center's (SDSC) Gordon Cluster through National Science Foundations Extreme Science and Engineering Discovery Environment (XSEDE).