DFT/TD-DFT Computations on Push-Pull Systems Featuring the Benzobisoxazole Core

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Asymmetric donor-acceptor benzobisoxazole dyes are of interest as push-pull systems due to their ease of synthesis and good optical properties. Strong donors and acceptors placed off of the core produce a large dipole and create the potential for intramolecular charge transfer in the excited state, which generally results in a narrow bandgap and emission in the near-infrared (NIR). While dyes that absorb in the visible region and emit in the NIR have potential in certain electronic devices (i.e. dye-sensitized solar cells) they are of particular interest in imaging and probing applications. The benzobisoxazole core is useful in that it allows for a modular synthesis of the final asymmetric dye and a large variation in the donor and acceptor moieties as the two ends are functionalized individually, producing numerous potential structures. Computational modeling of the energy levels of these molecules is quite beneficial. The calculations will help identify which moieties show the most promise and as a consequence will save our synthetic collaborators in the time and resources required for polymeric synthesis and characterization. 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*. 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).