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Dynamically Corrected Methods Can Explain Observed Discrepancies in Singlet Fission Properties of Quinoidal Bi- and Tetrathiophenes

MOHAMMAD R. MOMENI, Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota, Minneapolis, Minnesota 55455, United States — Quinoidal bithiophene has been introduced (*J. Phys. Chem. Lett.* **2015**, *6*, 1375) as a very promising isolated compound for intramolecular singlet fission (iSF). In contrast, another study (*J. Am. Chem. Soc.* **2015**, *137*, 11294) revealed that quinoidal tetrathiophenes have no activity in the iSF process and are strong fluorophores instead. To address this unprecedented discrepancy quinoidal bithiophene and tetrathiophene compounds and their derivatives are carefully examined using the CASPT2 technique. Through comparison of the CASPT2 results with the CASSCF and RAS-2SF data, it is found that the dynamic electron correlation present in the CASPT2 method plays a crucial role for correct description of the multiexciton nature of the triplet pair $^1[\text{TT}]$ state. Effects of substitution and structural modification on iSF activity of these compounds are also examined using the CASPT2 method where the obtained results are in accordance with previous experimental predictions. These results contribute to a better understanding of the iSF mechanism in quinoidal systems which could be relevant for designing new iSF active compounds.

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