# Supporting Information: Ground State Orbital Analysis Predicts $S_1$ Charge Transfer in Donor-Acceptor Materials

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## 1 Dimer-optimized vs. monomer-optimized structures

Figure S1 plots the absolute difference in $\eta$ for calculations performed with dimer-optimized vs. monomer-optimized structures. To clarify, dimer-optimized means that $\eta$ is computed for orbitals at their dimer-optimized geometries, i.e. monomer structures are not optimized. Monomer-optimized means that $\eta$ is computed between the dimer (at its optimized geometry) and monomers (at their optimized geometries). Alongside these absolute changes in $\eta$, we show changes in the atomic root mean squared deviation (RMSD) to indicate the magnitude of geometry change when comparing dimer-optimized and monomer-optimized structures. RMSD is calculated using the Cartesian coordinates of the systems, maximally overlapped via the Kabsch algorithm. See the main text for more information. Figure S1 shows correlation between the magnitude of structural changes (average atomic RMSD) and absolute difference in $\eta$.

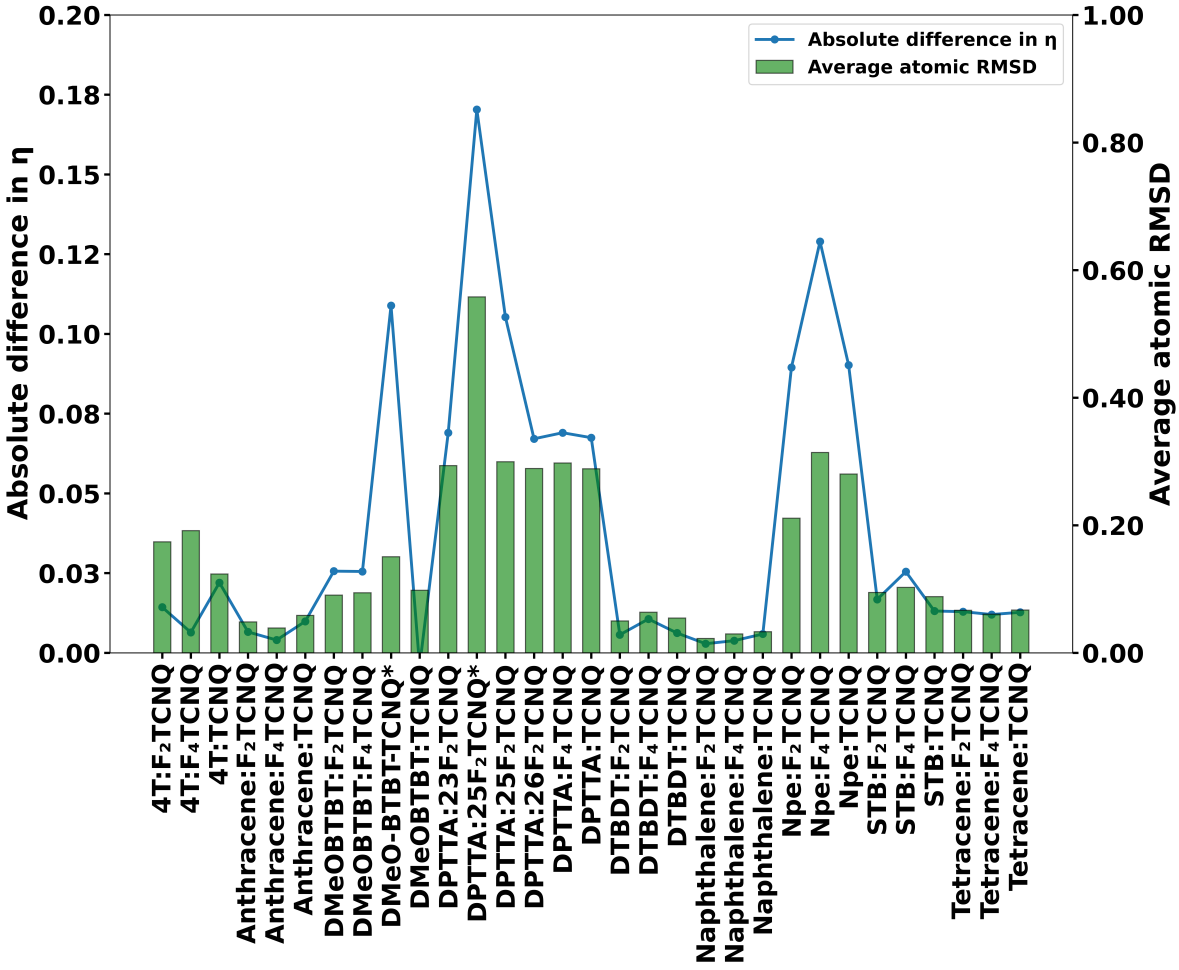


**Figure S1:** Plot of the absolute difference in $\eta$ overlaid with average atomic RMSD between the monomer-optimized and dimer-optimized geometries.