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First principles study of optical and electronic properties of anthradithiophene based organic conductors FAYE BARRAS, GUENTER SCHNEIDER, Oregon State University — Functionalized anthradithiophene (ADT) derivatives are high performance organic conductors where the addition of side groups such as triethylsilylethynyl (TES) to the ADT backbone induces a change in the morphology from a herringbone to a planar crystal structure in which improved intermolecular π-orbital overlap increases carrier mobility. Bulk type-II heterojunctions can be formed using matched pairs such as ADT-TES-F (donor) and ADT-TIPS-CN (acceptor). We report electronic and optical properties calculated from ab initio density functional theory (DFT) calculations for ADT derivatives. Exciton and exciplex formation and charge separation in ADT bulk heterojunctions is studied using 2 molecule model calculations for ADT-TES-F (donor) and ADT-TIPS-CN or C_{60} (acceptor). We compare our results to available experimental results such as photo luminescence and photocurrent measurements.

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