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First principles study of optical and electronic properties of anthradithiophene based organic conductors FAYE BARRAS, GUENTER SCHNEIDER, Oregon State University — Electronic band structures based on first principles density functional theory are reported for functionalized anthradithiophene (ADT) derivatives, such as ADT-TES-F (donor) and ADT-TIPS-CN (acceptor).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. A comparison of the band gaps and effective masses deduced from theoretical calculations may indicate which side groups promote increased optical response and electrical conduction. We compare our results to available experimental results such as photoluminescence and photocurrent measurements.

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