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Analysis of Metallic Conduction at the Interface of TTF and TCNQ Crystals[1] VIKTOR ATALLA, Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, MINA YOON, ORNL, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin — Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing electronic phenomena while being environmentally friendly, low cost, and mechanically flexible. Here we study the donor/acceptor interface of TTF and TCNQ organic molecular crystals which was found to exhibit metallic conduction whereas the individual crystals are large band-gap semiconductors. Using density functional theory (DFT) we first compare the performance of different exchange-correlation (XC) functionals for TTF and TCNQ dimers. All employed XC functionals consistently give electron transfer from TTF to TCNQ and the van der Waals (vdW) corrected molecular binding distances are within ≈ 0.1 Å of the MP2 value, indicating that within DFT the system can be qualitatively described by semilocal functionals. We construct interfaces between the two types of crystals and calculate their electronic structures. On a PBE + vdW level we find indications for metallic conduction at the interface, due to metallic bands that are exclusively induced from the interface layers of TTF and TCNQ molecules.

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