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**A Theoretical Investigation of the Charge Transfer System TCNQ-F4 and Alpha-Sexithiophene** KAI-FELIX BRAUN, SAW-WAI HLA, Nanoscale & Quantum Phenomena Institute, Physics & Astronomy Dept., Ohio University, Athens, OH 45701 — The electronic and geometrical structures of the charge-transfer system of alpha-sexihiophene and tetrafluorotetracyanoquinodimethane are calculated self-consistently from first principles. By means of density functional theory (DFT) methods several configurations of the free molecules are calculated within LDA and B3LYP employing a plane wave basis and different atomic orbital sets. The combined system exhibits preferential binding of the center of the TCNQ-F4 on top of a c-c bond of the sexithiophene, thereby the central configuration having the lowest energy. As opposed to the periodic arrangement in a crystal of the related system dimethylquaterthiophene and TCNQ-F4, the free system exhibits a strong interaction going along with a substantial polarization of both molecules. For comparison with scanning tunneling spectroscopy results, the molecules were adsorbed in a parallel geometry on a Au(111) slab. To take into account the voltage applied to the STM tip the system was finally calculated within an electric field. This work is financially supported by the US-DOE grant no. DE-FG02-02ER46012.

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