Effect of 2,3,5,6-Tetrafluoro-7,7,8,8tetracyanoquinodimethane Charge Transfer Dopants on the Conformation and Aggregation of Poly(3-hexylthiophene)

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SUPPORTING INFORMATION



Fig. S1. Raman spectra for (thiophene)₄, F_4 -TCNQ, Complex I and Complex II calculated from DFT. The isolated molecules and complex I are calculated at B3LYP/6-311++G*, complex II are calculated at the B3LYP/6-31++G* level.

Raman spectra of an oligothiophene surrogate for P3HT and F_4 -TCNQ are simulated from DFT (model described in main text).



Fig. S2. Absorption and emission spectra for P3HT nanofiber (NF) made from A, C) anisole and B, D) toluene solvents. Black lines are the spectra from pristine NF. Grey lines are the spectra from NF with F_4 -TCNQ doping. Absorption spectra A, B) are normalized by 0-0 peaks. Emission spectra C, D) were taken from the samples with same O. D. values.



Fig. S3. STEM/EELS images of P3HT/PCBM films without (top panels) and with 5% F_4 -TCNQ doping. Left; relative carbon/sulfur signal, right; sulfur signal.