Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Tuning the Seebeck coefficient of naphthalenediimide by electrochemical gating and doping

Qusiy H. Al-Galiby,[a,b*], Hatef Sadegi,[a] David Zsolt Manrique,[c] and Colin J. Lambert[a*]

[a]Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom.
[b]Department of Physics, College of Education, University of Al Qadisiyah, 58002, IRAQ.
[c]Department of Electronic & Electrical Engineering - Photonics Group, University College London, United Kingdom.

*Corresponding author: c.lambert@lancaster.ac.uk and qusiy.algaliby@qu.edu.iq

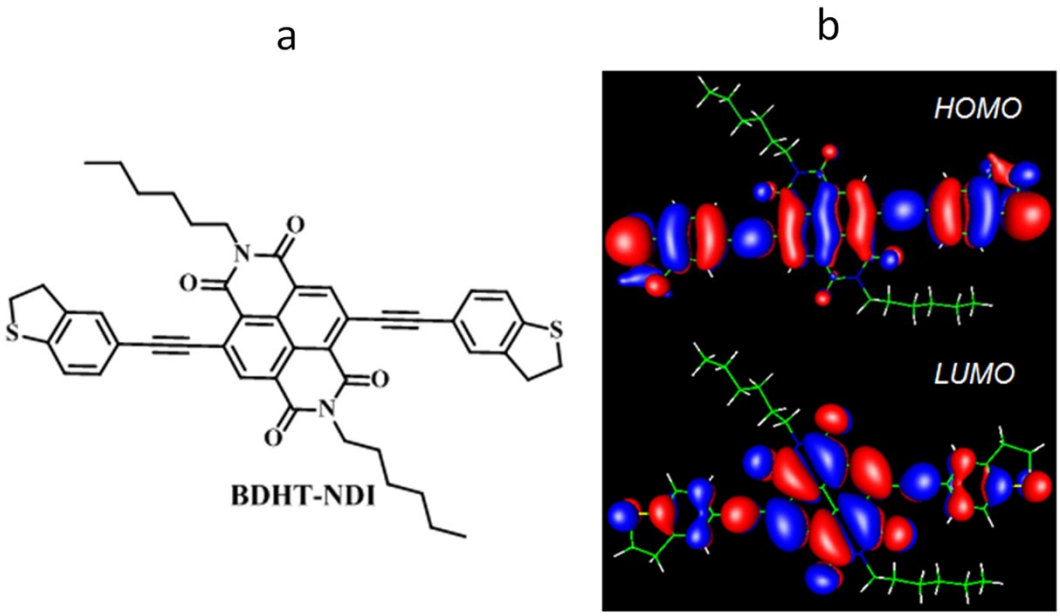

Figure S1. The left figure 1a shows the chemical structure of BDHT-NDI molecule, the right figure 1b shows Iso-surfaces of frontier molecular orbitals of NDI molecule obtained using DFT. Red corresponds to positive and blue to negative regions of the wave functions.

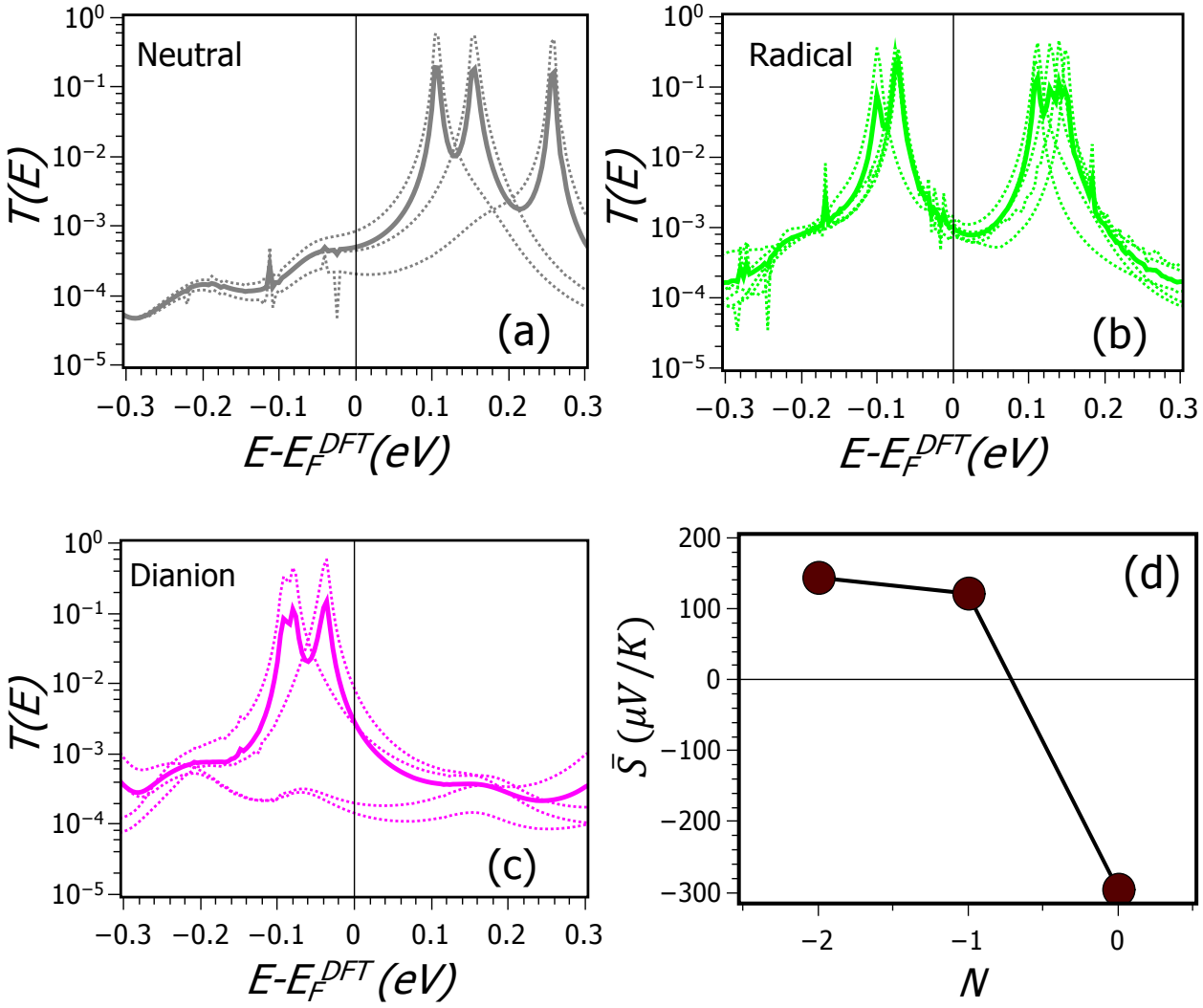

Figure S2. (a) Transmission curves for junction geometries with double layers located at distances y=5Å, y=5.8Å and y=4.05Å, respectively. The continuous curves are the averaged transmission coefficients $\bar{T}(E)$ and the dotted curves show the transmission coefficients for different charge double layer arrangements. Figure 4d shows the average room-temperature thermopower $\bar{S}$ for three redox states obtained using DFT-predicted Fermi energy E_F^{DFT}. The colour code refers to the three different states, NDI-N (black), NDI-R (blue) and NDI-D (red).

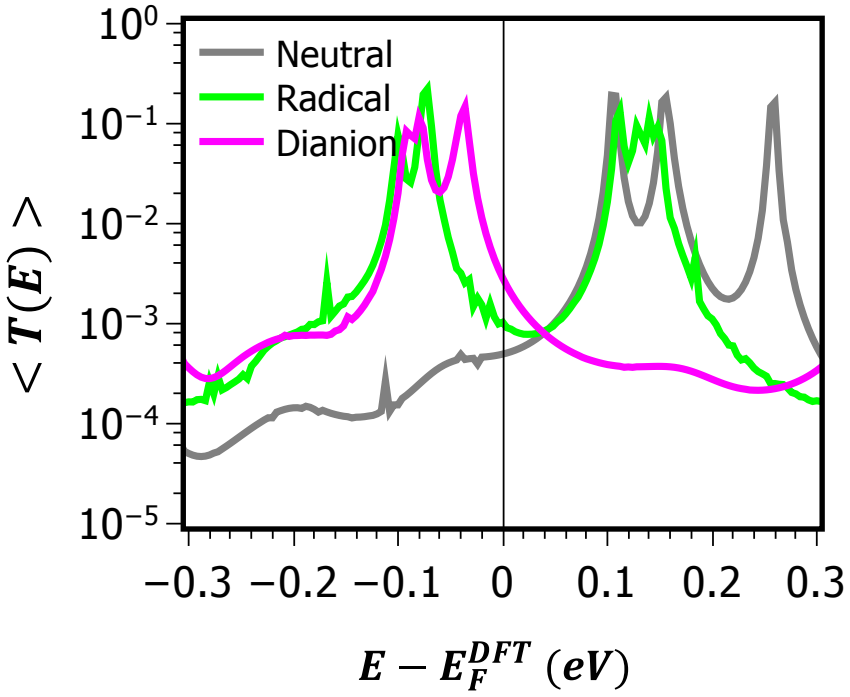

Figure S3. The corresponding ensemble-averaged tranmsission coefficients corresponding to Figure 3 of the main text

NDI doping with TTF:

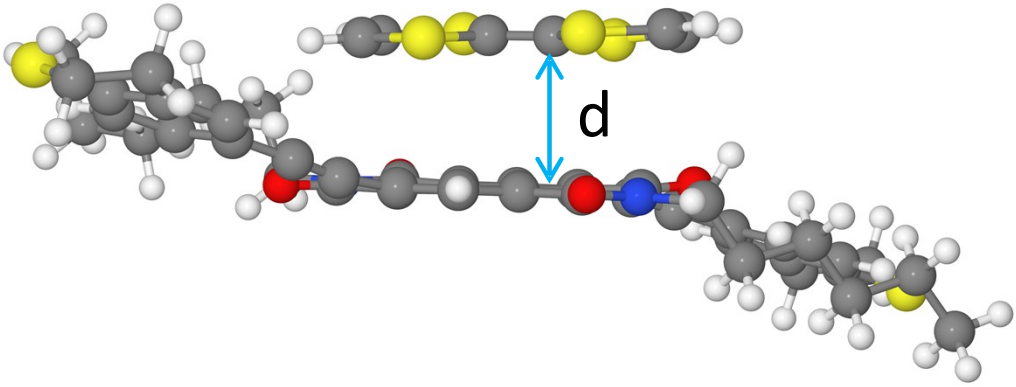

Figure S4: Optimised configurations for TTF bonded to the NDI molecule.

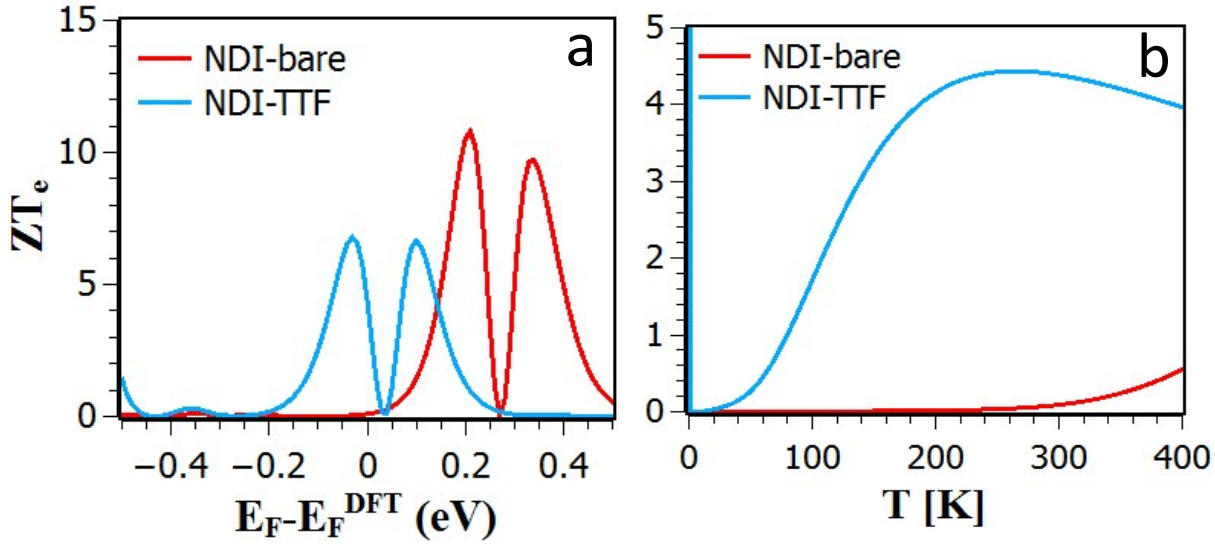

Figure S5. (a) Room-temperature- electronic contribution to figure of merit ZT_e versus Fermi energy for bare and TTF-doped NDI. (b) Electronic contribution to figure of merit ZT_e versus temperature, evaluated using the DFT-predicted value of the Fermi energy.

NDI doping with TCNE:

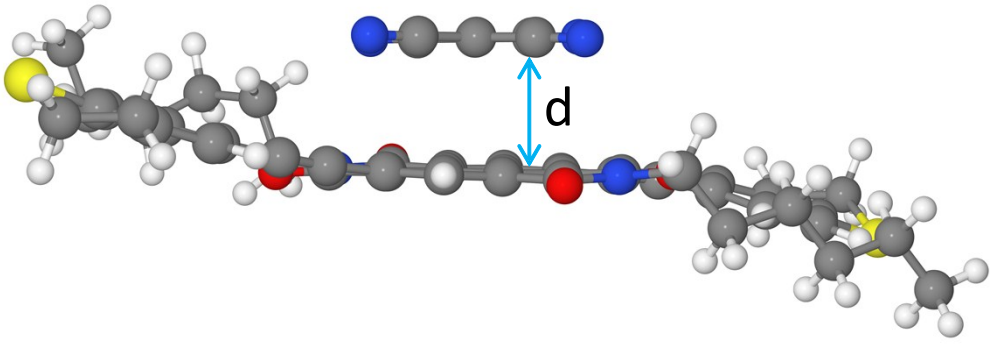

Figure S6: Optimised configurations for TCNE bonded to the NDI molecule.

Table S1: DFT results for the number ΔN of electrons transferred to the TCNE, the binding energy ΔE of the TCNE to the NDI molecule and optimal distance of the TCNE from the NDI.

	ΔN	*ΔE (eV)*	*D (Å)*
TCNE	-0.217	-0.288	3.85

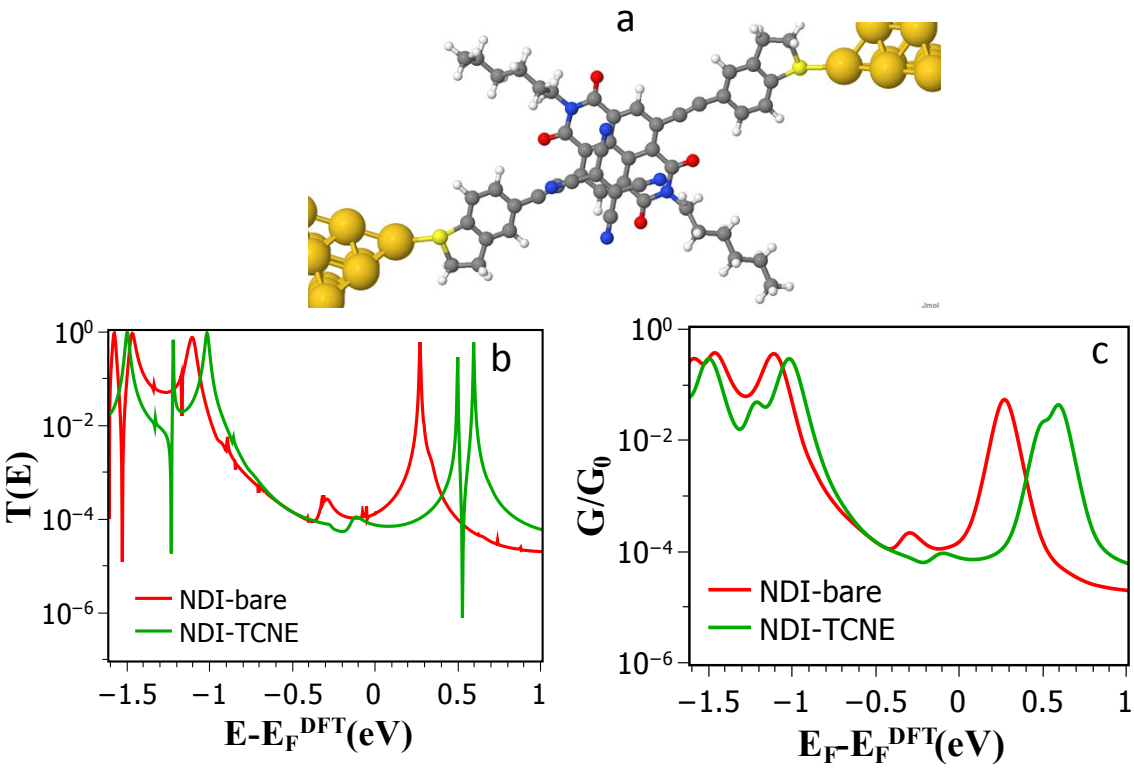

Figure S7. (a) An NDI molecule complexed with TCNE. (b) Transmission coefficients as a function of energy for the NDI (red) and NDI-TCNE (green). (b) Room-temperature electrical conductance for the bare NDI (red) and NDI-TCNE (green).

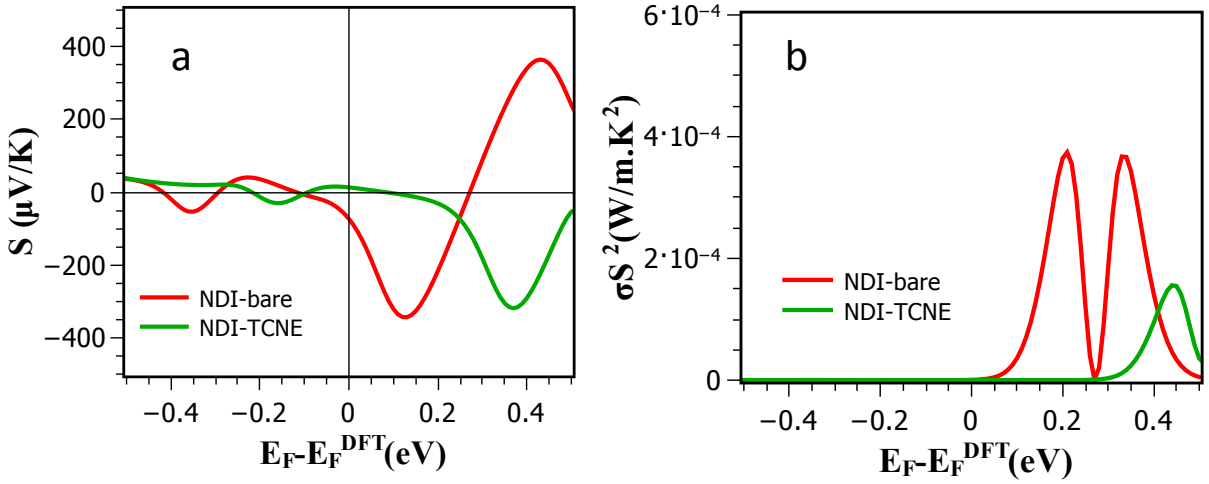

Figure S8. Room-temperature Seebeck coefficients and power factors versus Fermi energy for bare and TCNE-doped NDI.