Supplementary Information
for

$C_{60}ThSe_2$/ITO interface formation: photoemission – based charge transfer recognition for organic electronics application

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Cyclic Voltammetry

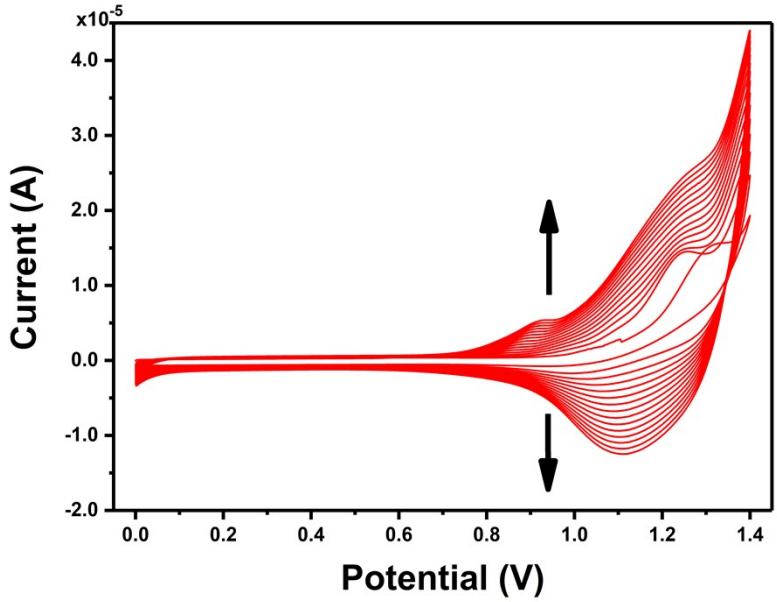

Fig.S1. CV curve recorded in 0.1 mM solution $C_{60}ThSe_2$ in 0.2 M Bu_4NBF_4/CH_2Cl_2 with ITO as a working electrode, 15 scan cycles, scan rate: 0.1 V/s.

Fig.S1 presents the CV curve recorded in $C_{60}ThSe_2$ solution with ITO acting as a working electrode. Similarly to our previous studies on the terthiophene-fullerene dyads [1], the irreversible oxidation is observed at ca. 1.3 V, that arises from the oxidation of organic unit initiating the electropolymerization process. Further sweeping of the potential reveals the new redox couple at ca. 1.1 V and causes the continuous increase in the recorded current. These together confirm the

polymerization of $C_{60}ThSe_2$ dyad and the simultaneous deposition of the conjugated polymeric film on the ITO surface.

UV-VIS Spectroscopy

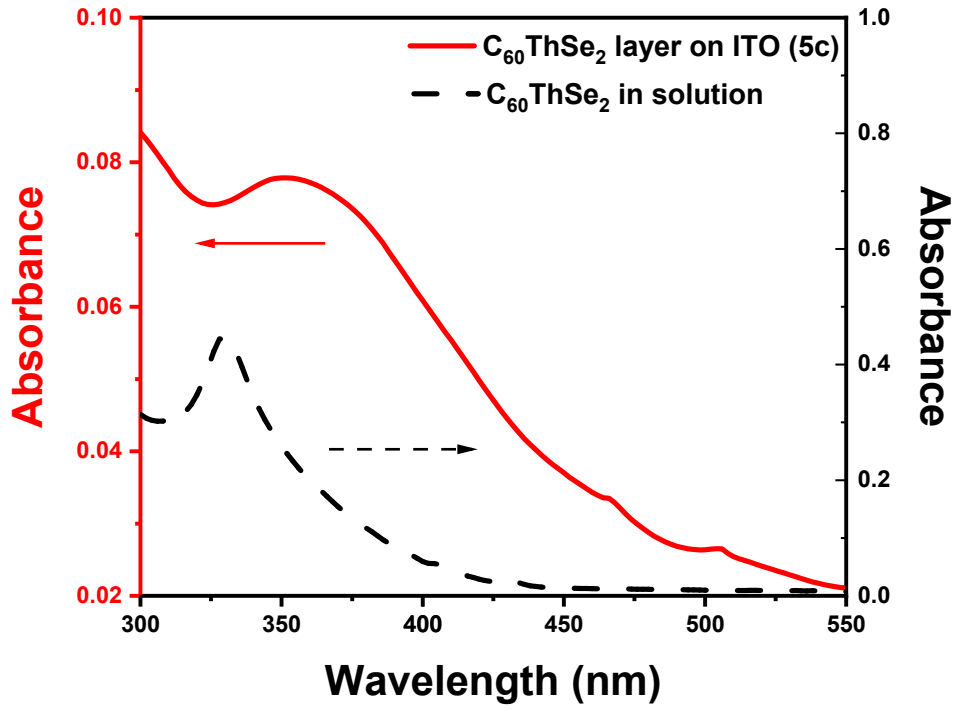

Fig.S2. UV-Vis spectra of $C_{60}ThSe_2$/ITO (5c) (red solid line) and $C_{60}ThSe_2$ in dichloromethane (black dashed line). In the case of UV-Vis spectrum of the layer, ITO was used as a reference, while in the case of $C_{60}ThSe_2$ solution – dichloromethane.

UV-Vis spectra of electrochemically deposited $C_{60}ThSe_2$ layer, given in Fig.S2, show one broad absorption band with maximum at ca. 360 nm, arising from the fullerene and conjugated polymeric chain ($\pi \rightarrow \pi^*$ transition) absorption [1]. The recorded band is significantly broaden with onset being batochromically shifted when compared with the UV-Vis spectrum of $C_{60}ThSe_2$ dyad in solution, indicating the elongation of the conjugated chain [2]. The onset of the absorbance band, and thus the calculated optical band gap, was steadily increasing with the increase in the number of electropolymerization cycles (Table S1).

Tab. SI 1. Optical data

Sample set	λ_{onset}/ nm	Optical band gap E_g/ eV
5c	465	2.67
10c	484	2.56
15c	493	2.52

**Optical band gap E_g=1240/ λ_{onset}*

References

[1] A. Blacha-Grzechnik, M. Krzywiecki, R. Motyka, Electrochemically Polymerized Terthiopehene − C60 Dyads for the Photochemical Generation of Singlet Oxygen, J. Phys. Chem. C. 123 (2019) 25915–25924. https://doi.org/10.1021/acs.jpcc.9b06101.

[2] B. Lu, S. Zhen, S. Ming, J. Xu, G. Zhao, RSC Advances, (2015) 70649–70660. https://doi.org/10.1039/c5ra11849b.