

Unravelling the role of electron-hole pair spin in exciton dissociation in squaraine-based organic solar cells by magneto-photocurrent measurements

Maciej Klein*, Sayani Majumdar, Paweł Zassowski, Waldemar Stampor

* mklein@mif.pg.gda.pl

Spectroscopic measurements

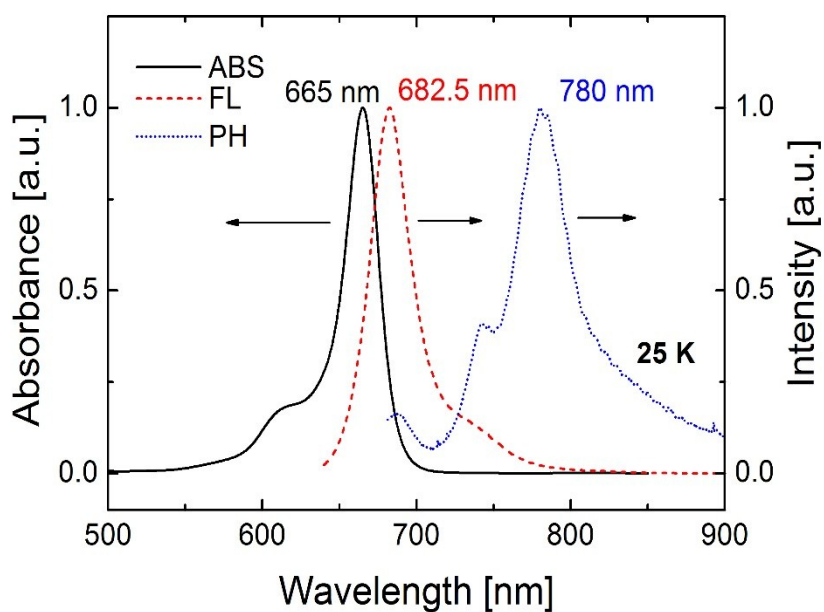


Figure S1. Absorbance - ABS, fluorescence - FL (both measured at room temperature) and phosphorescence - PH (measured in 25 K) spectra of SQ2 molecule dissolved in 1,2-dibromoethane

EPR measurements

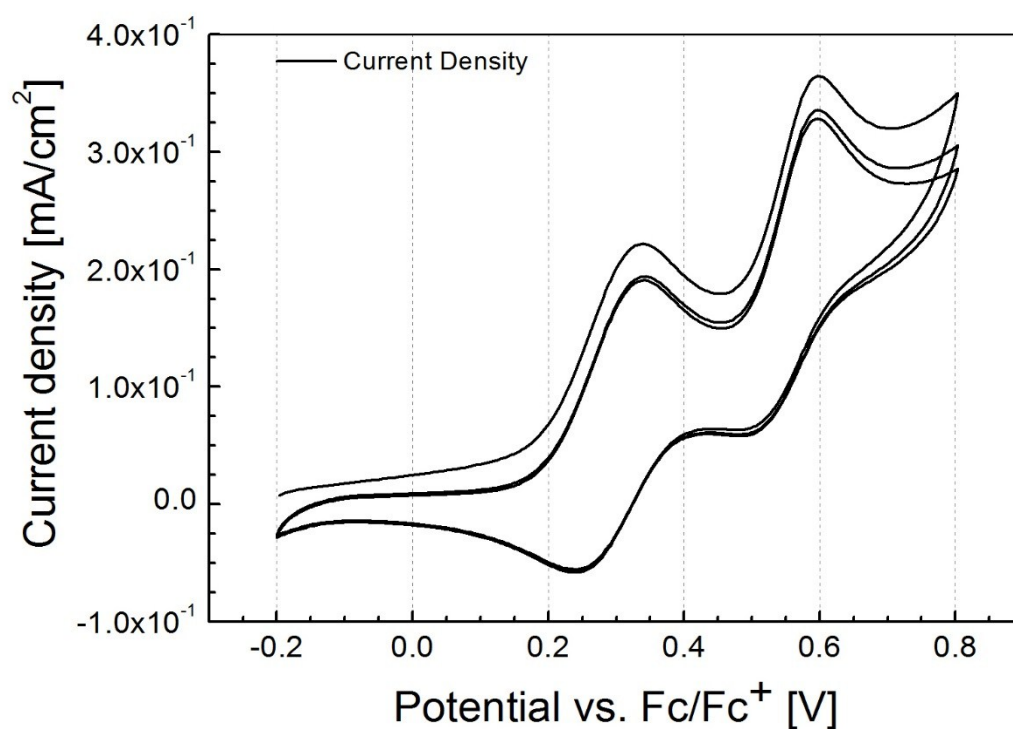


Figure S2. Cyclic voltammogram of SQ2. Measurements conditions: 1 mM solution of SQ2 in 0.1 M dichloromethane/tetrabutylammonium hexafluorophosphate electrolyte, scan rate: 100 mV/s

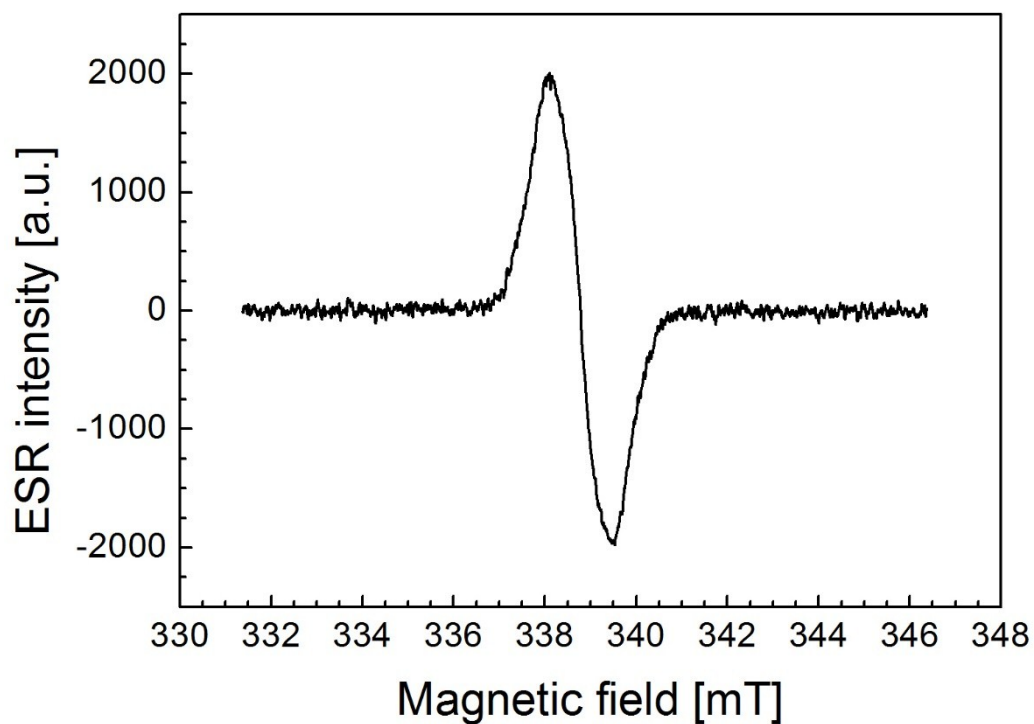


Figure S3. EPR spectra of radical cation of SQ2, recorded in-situ during oxidation

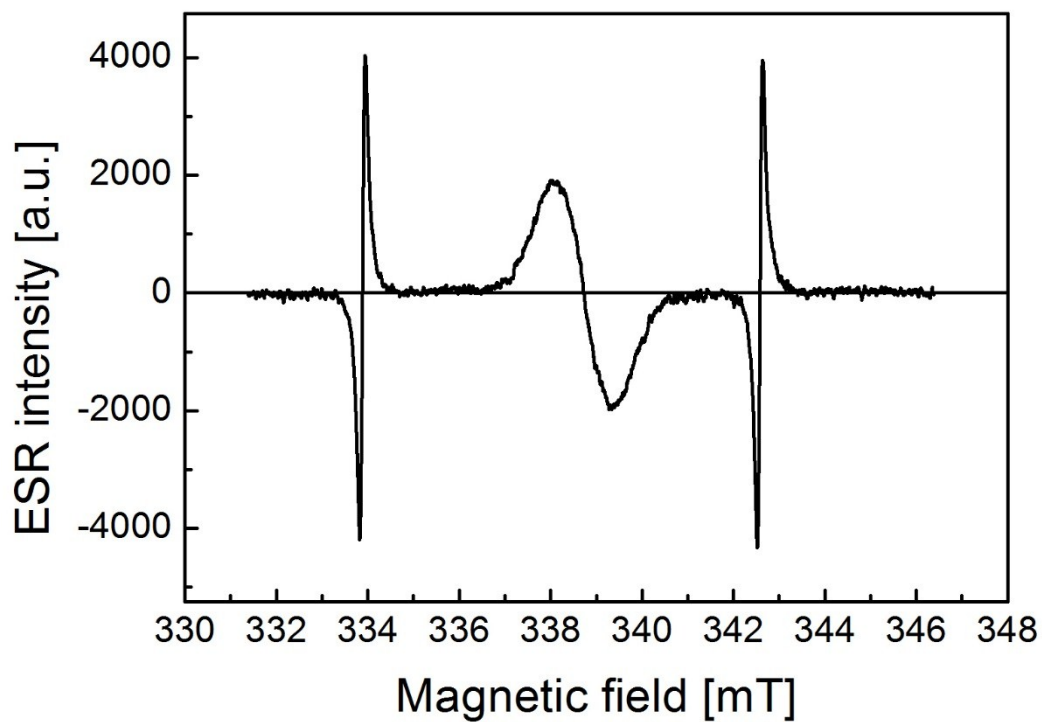


Figure S4. EPR spectra of radical cation of SQ2, recorded in-situ during oxidation at potential of 0.3 V vs. Fc/Fc⁺. Measurement conditions: microwave power: 2 mW, modulation width: 0.1 mT. Two sharp lines on the sides of the spectrum correspond to the g factor internal standard of the spectrometer

AFM measurements

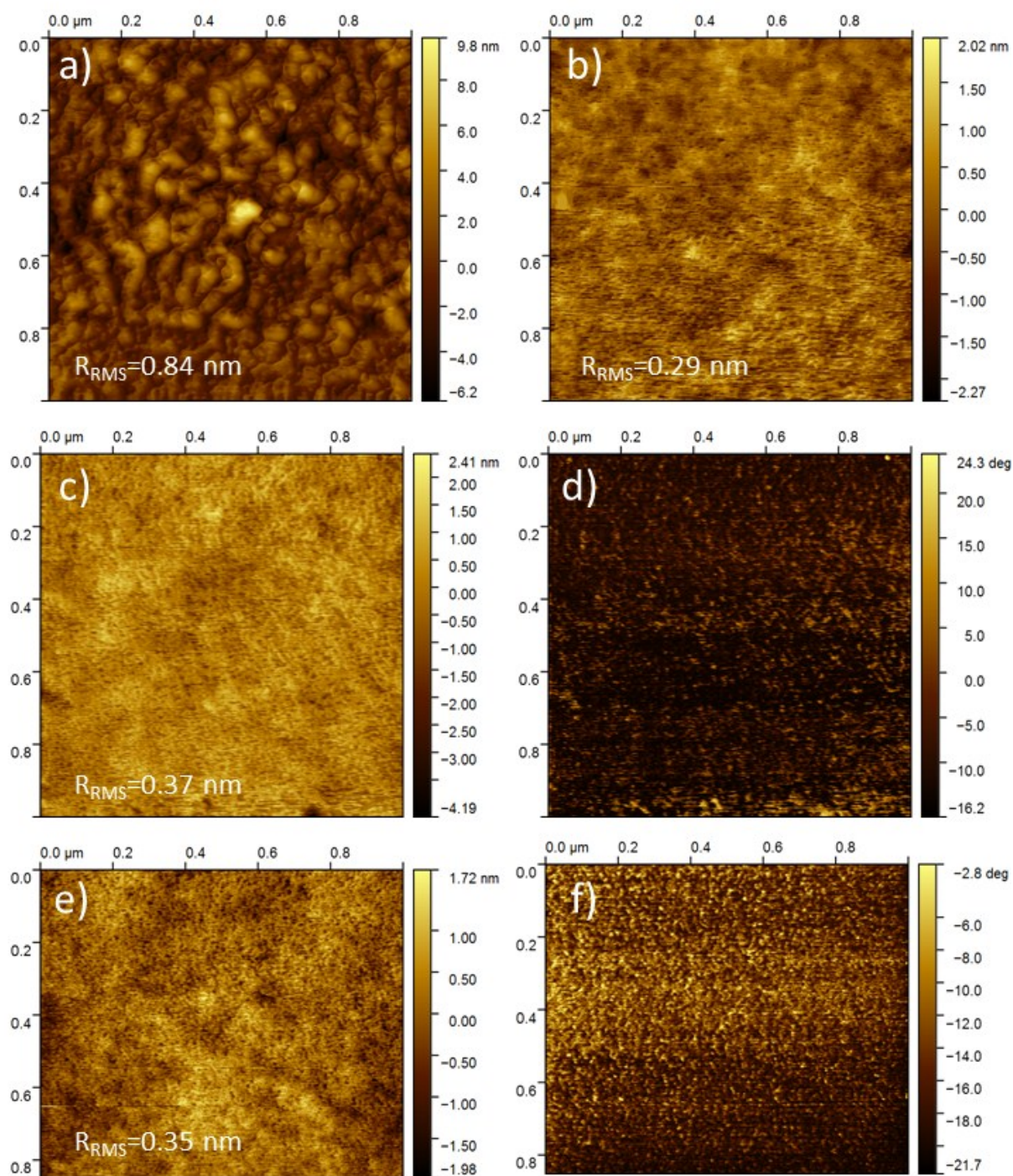


Figure S5. AFM topography scans of thermally evaporated MoOx thin film (a) and spin-coated: pristine SQ (b), SQ:PC₆₀BM 1:10% (c) and SQ:PC₆₀BM 1:6 (e) thin films. R_{RMS} as the insets represent root mean square roughness value measured across the scan. Phase separation images of spin-coated SQ:PC₆₀BM 1:10% (d) and SQ:PC₆₀BM 1:6 (f) thin films

Fitting parameters of MPC lineshapes

Table S1. The parameters used for the Lorentzian fitting shown in Figure 2a. A_{LFE} and B_{LFE} denote the amplitude and the half width ($B_{1/2}$) at half signal maximum, respectively, for low-field (LFE) and medium-field (MFE) effects.

Temperature [K]	A_{LFE} [-]	B_{LFE} [mT]	A_{MFE} [-]	B_{MFE} [mT]
200	1.2	3	1.2	30
290	0.465	4	-	-

Table S2. The parameters used for the Lorentzian fitting shown in Figure 3a. A_{LFE} and B_{LFE} denote the amplitude and the half width ($B_{1/2}$) at half signal maximum, respectively, for low-field (LFE) effects.

Active layer	A_{LFE} [-]	B_{LFE} [mT]
SQ	0.465	4
SQ:PCBM (1:0.1%)	0.39	4
SQ:PCBM (1:10%)	-0.2	4
SQ:PCBM (1:6%)	-0.105	8

Table S3. The parameters used for the Lorentzian fitting shown in Figure 3b and Figure 4a. A_{LFE} and B_{LFE} denote the amplitude and the half width ($B_{1/2}$) at half signal maximum, respectively, for low-field (LFE) and high-field (HFE) effects according to the single- and double-Lorentzian functions.

Temperature [K]	A_{LFE} [-]	B_{LFE} [mT]	A_{HFE1} [-]	B_{HFE1} [T]	A_{HFE2} [-]	B_{HFE2} [T]
200	-0.27	4	1.7	1.4	5	20
250	-0.225	7	1.2	1.6	5.5	15
290	-0.105	8	1.1	2	5.5	15

Table S4. The parameters used for the KWW fitting shown in Figure 4b. τ represent an average relaxation time of CT states and α is the dispersive parameter.

Temperature [K]	α [-]	τ [ns]
200	0.51	1.88
250	0.5	1.02
290	0.61	0.57