

Supporting Information Materials for Second Generation of Diketopyrrolopyrrole Dyes for NiO Based Dye-Sensitized Solar Cells

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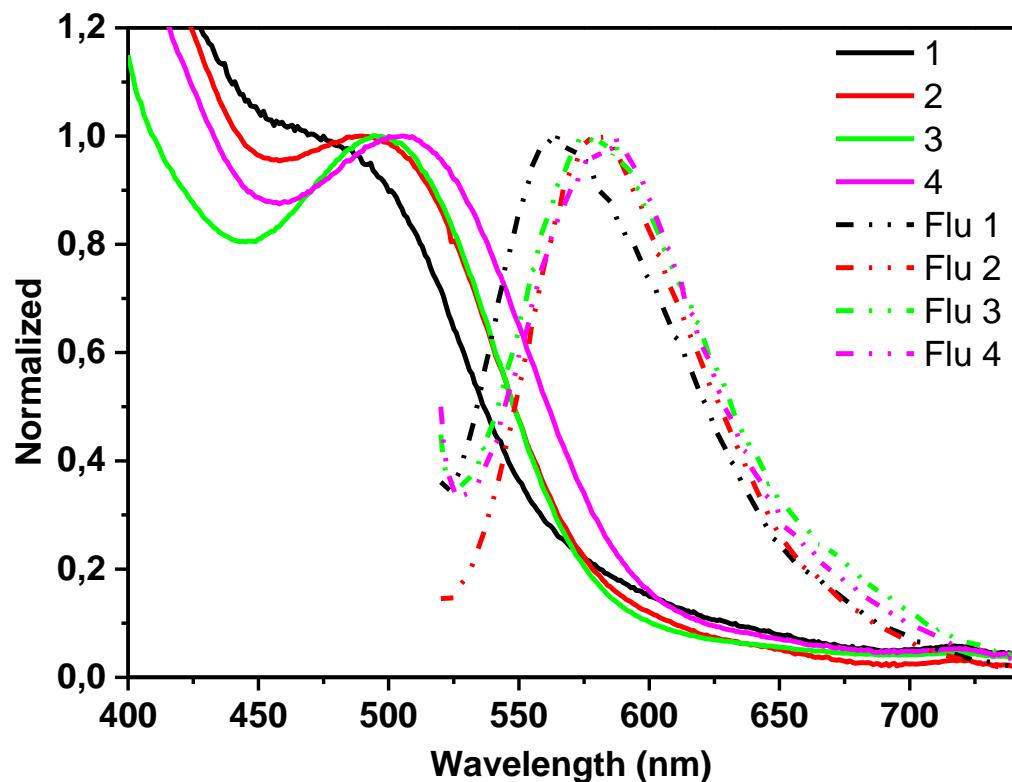


Figure S1. Normalized UV-vis absorption (solid) and emission (dashed) for 1-4 sensitized on NiO.

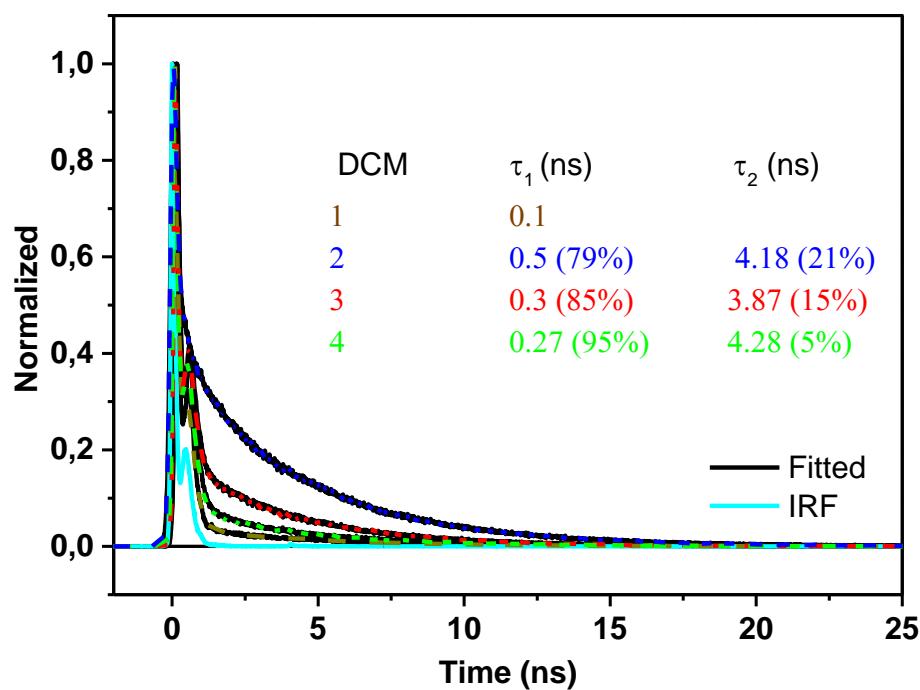


Figure S2. Normalized TCSPC results with time constants for each dye in DCM.

Table S1. Time constants from global fits of femtosecond TA data for **1-4** in DCM

Dyes	τ_1/ps	τ_2/ps	τ_3/ps	τ_4/ps
1	0.76 ± 0.062	26 ± 7	144 ± 23	(>2000 ps) ^a
2	0.61 ± 0.24	17.8 ± 5.7	732 ± 158	>2000 ps
3	1.13 ± 0.51	16.2 ± 4.8	142 ± 35	(>2000 ps) ^a
4	0.96 ± 0.46	12.1 ± 3.2	63.3 ± 21.5	(>2000 ps) ^a

^arepresents <5% of the amplitude at all wavelengths.

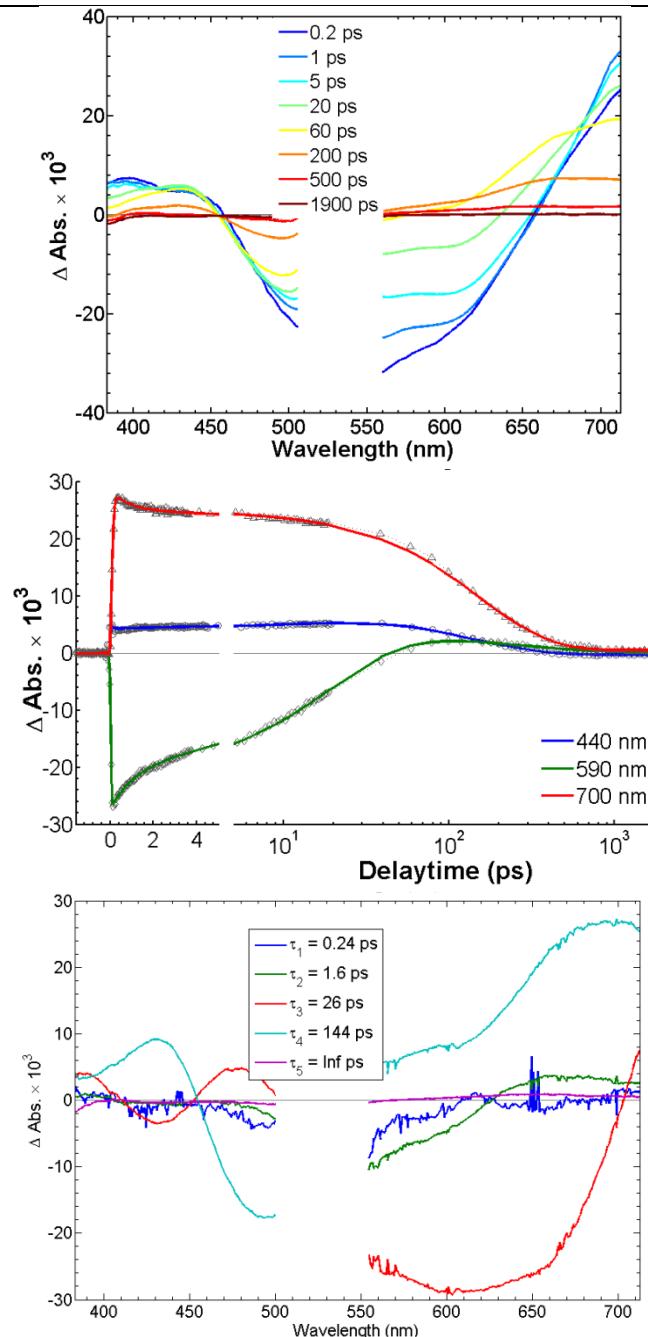


Figure S3. Transient absorption spectra (up), kinetic traces at certain wavelength (middle) and Decay associated spectra (DAS) from global fit (bottom) of **1** in DCM.

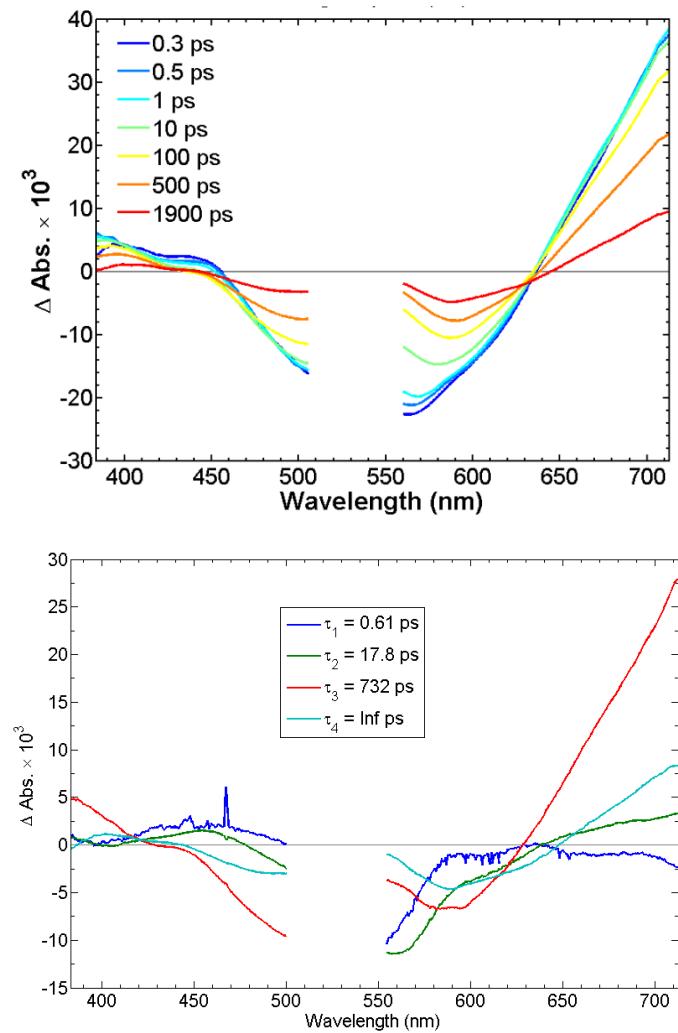


Figure S4. Transient absorption spectra and Decay associated spectra (DAS) from global fit of **2** in DCM.

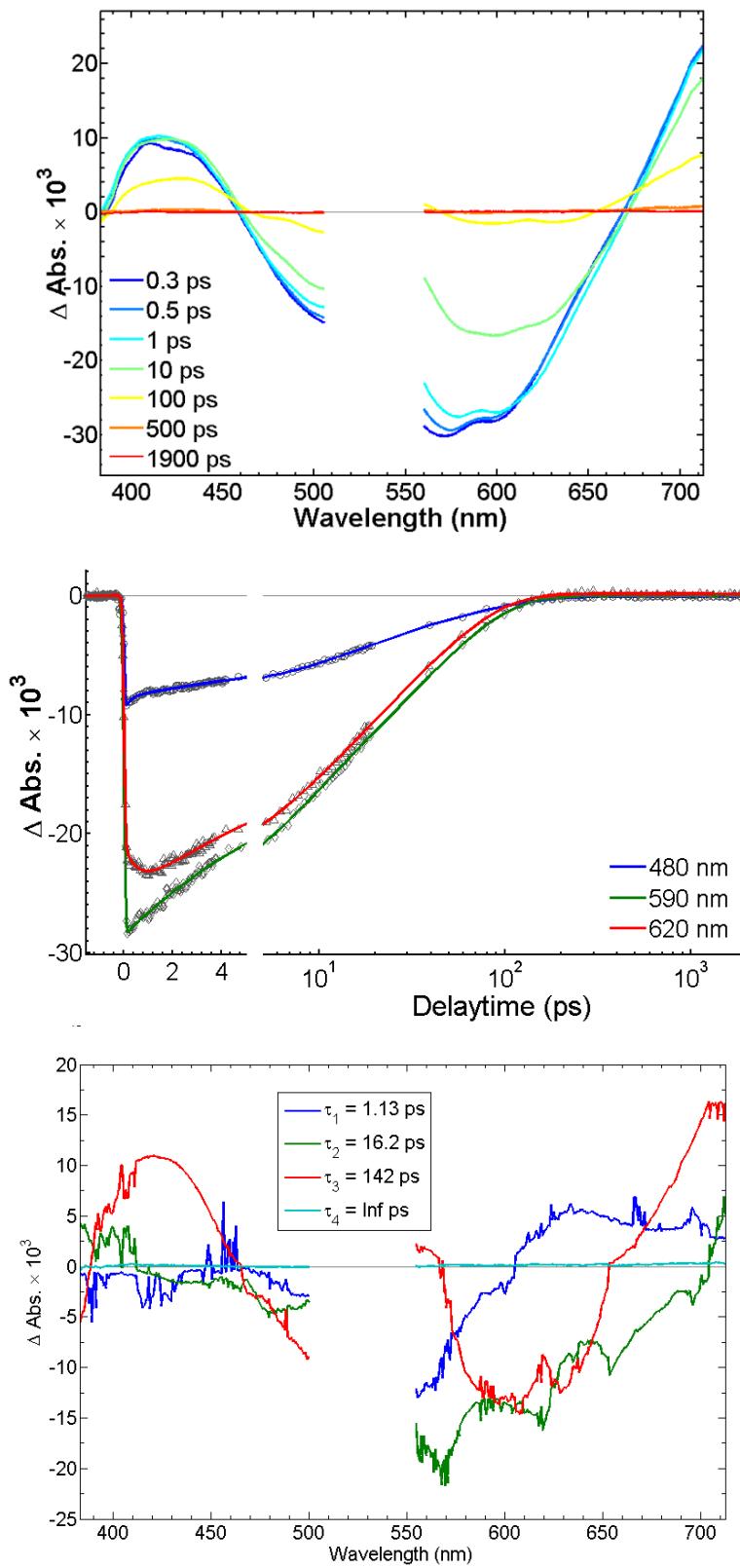


Figure S5. Transient absorption spectra (up), kinetic traces at certain wavelength (middle) and Decay associated spectra (DAS) from global fit (bottom) of **3** in DCM.

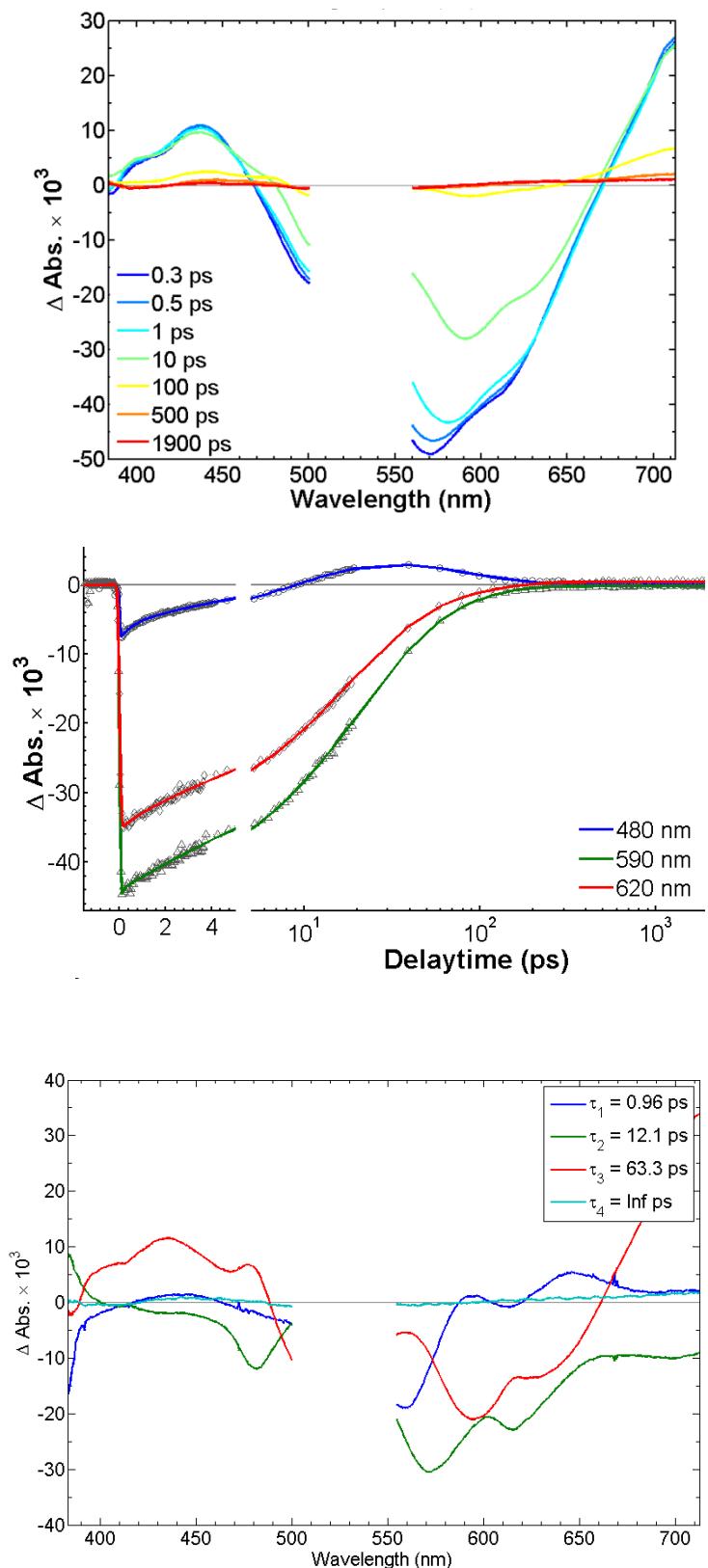


Figure S6. Transient absorption spectra (up), kinetic traces at certain wavelength (middle) and Decay associated spectra (DAS) from global fit (bottom) of **4** in DCM.

Table S2. Time constants from global fits of femtosecond TA data for **1-4** on NiO

Dyes	τ_1/ps	τ_2/ps	τ_3/ps	τ_4/ps	τ_∞
1	0.16 ± 0.12	0.82 ± 0.53	9.21 ± 4.52	61 ± 45	<1% amplitude at all wavelengths
2	0.18 ± 0.09	1.21 ± 0.64	6.8 ± 5.6	57 ± 37	<1% amplitude at all wavelengths
3	0.23 ± 0.067	1.69 ± 0.34	12.5 ± 4.7	290 ± 18	Large amplitude at all wavelengths
4	0.2 ± 0.1	1.3 ± 0.5	14.1 ± 5.9	242 ± 28	Large amplitude at all wavelengths

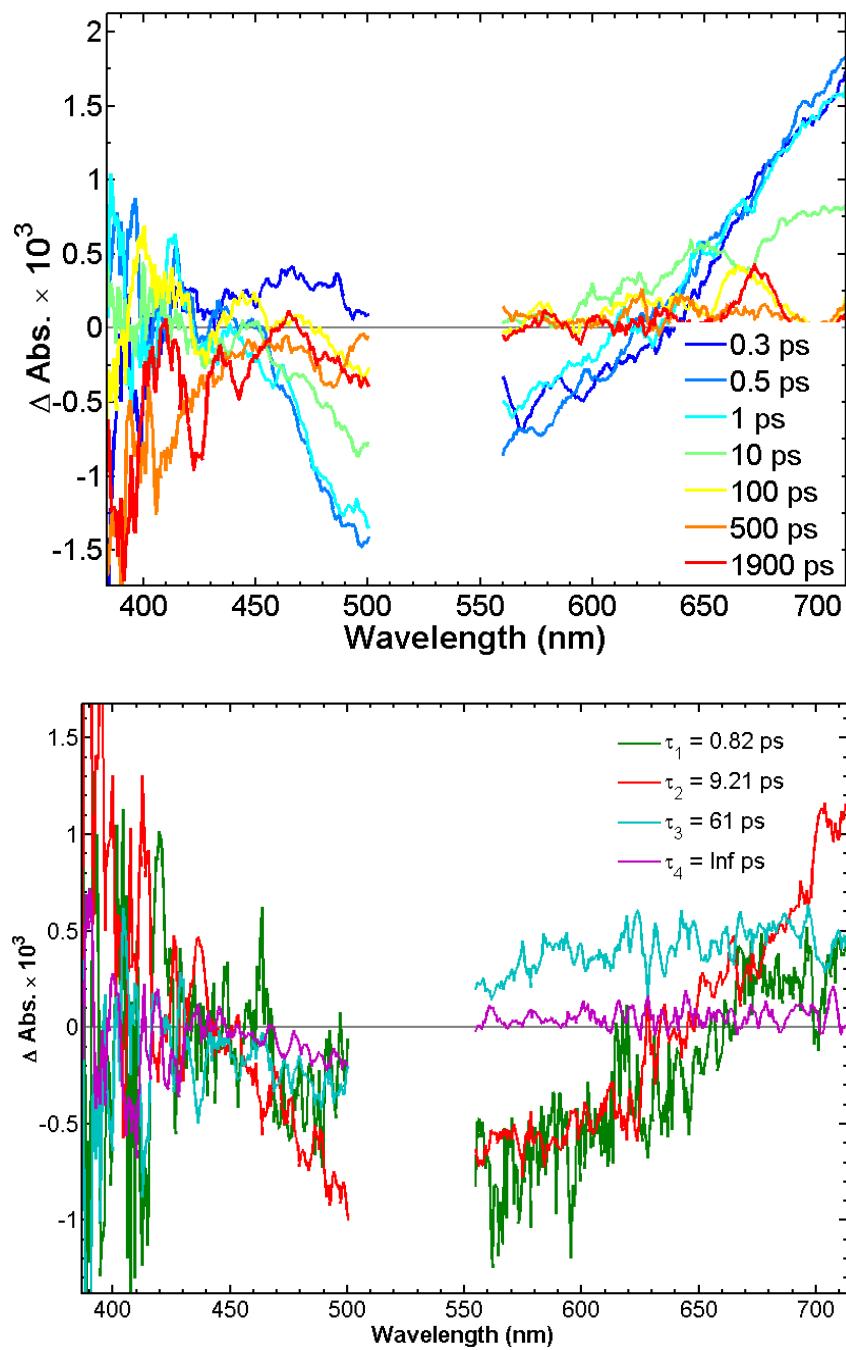


Figure S7. Transient absorption spectra and Decay associated spectra (DAS) from global fit of NiO/1.

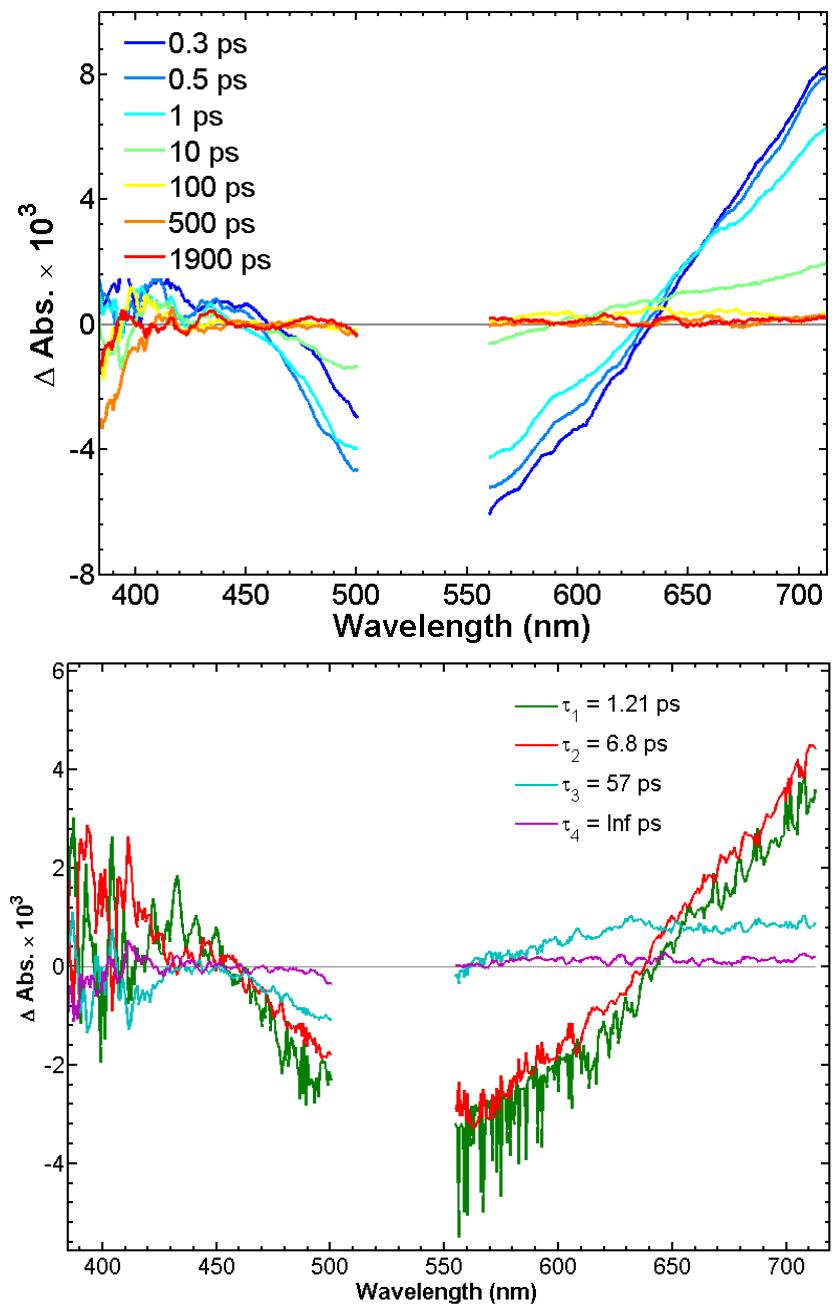


Figure S8. Transient absorption spectra and Decay associated spectra (DAS) from global fit of NiO/2.

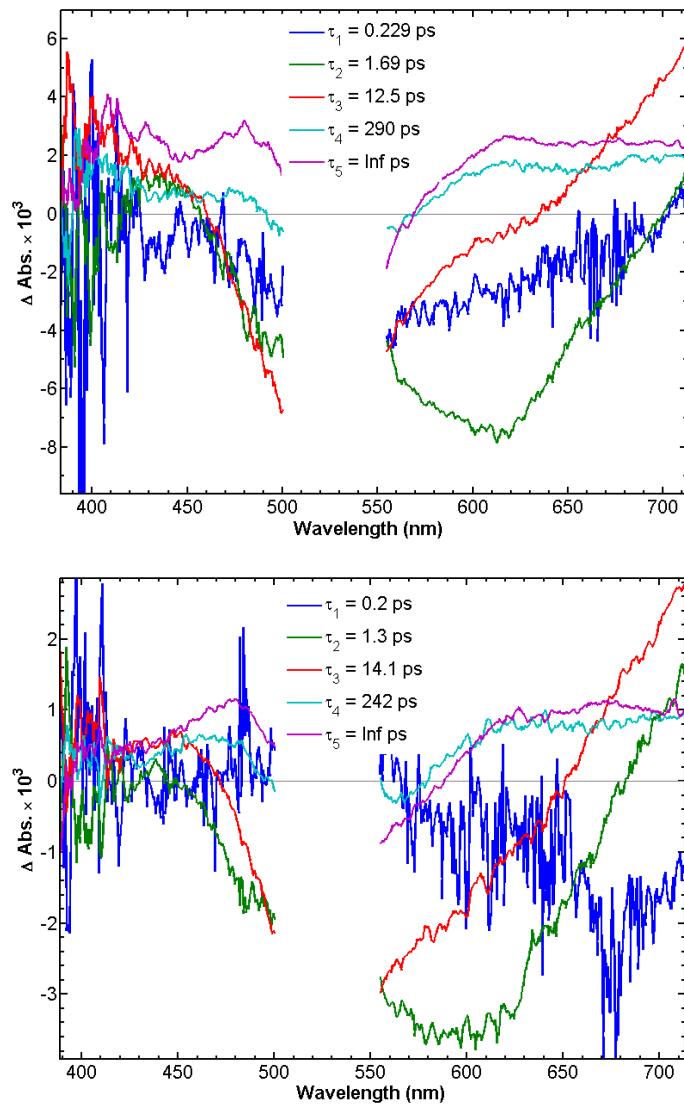


Figure S9. Decay associated spectra (DAS) from global fit of NiO/3 (up) and NiO/4 (down).

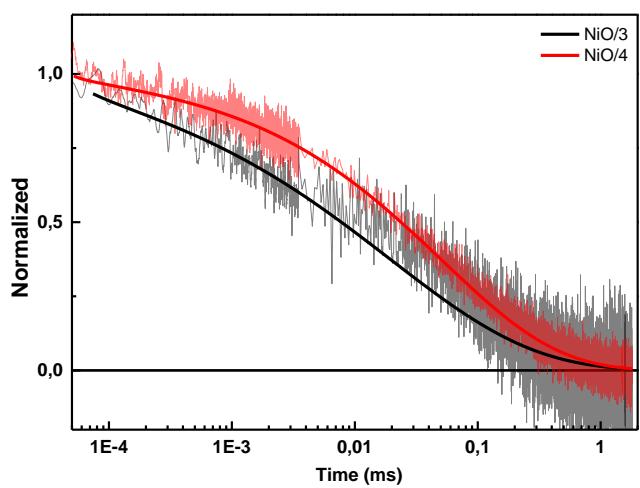


Figure S10. NiO/3 (gray) and NiO/4 (red) reduced state transient absorption as a function of time in presence of LiClO₄ (Excitation at 532 nm). The smooth lines are stretched-exponential fits (KWW), which do not fit that well, especially not for **3**.

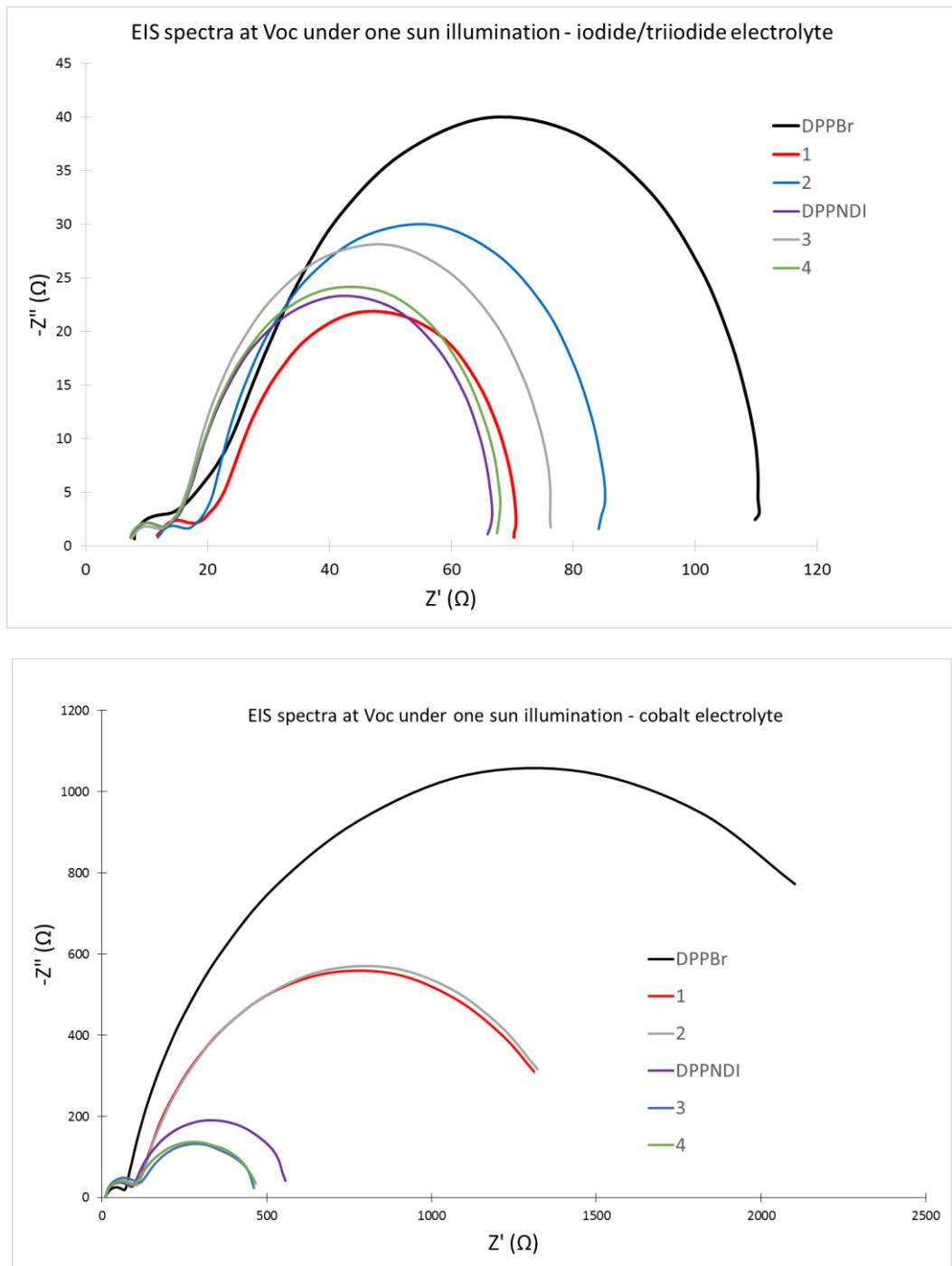


Figure S11. Nyquist plots of NiO based p-DSSC recorded with iodide electrolyte (up) and cobalt electrolyte (down) recorded under illumination at V_{oc} .

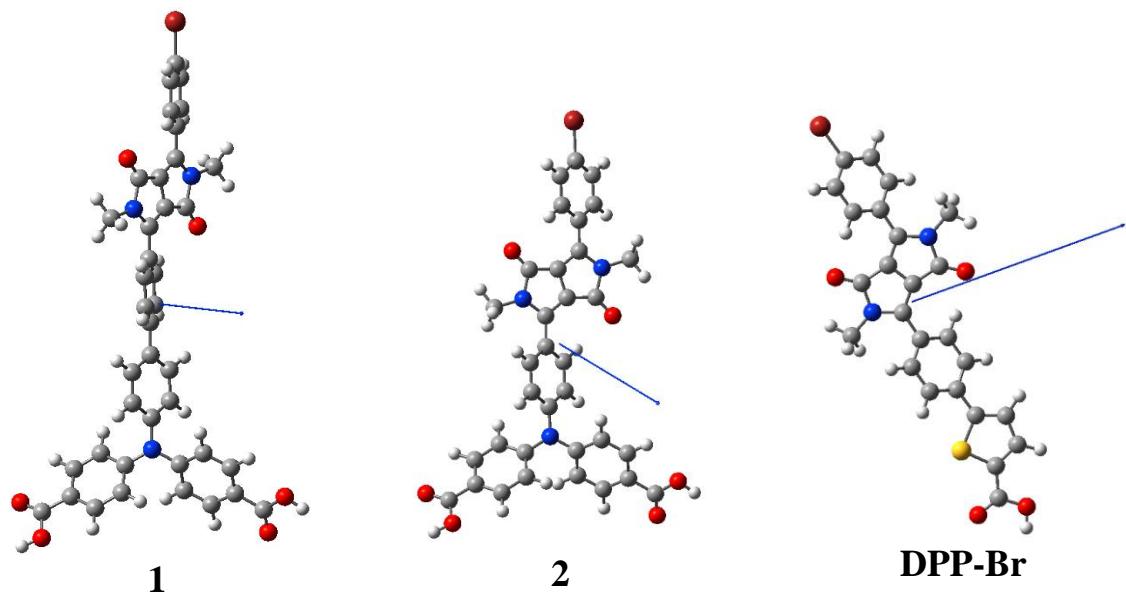


Figure S12. Representation of the permanent dipole moment of the dyes **1**, **2** and **DPP-Br**. The point of the arrow indicates the highest positive charge density.