SUPPORTING INFORMATION

Record power conversion efficiencies for Iron (II)-NHC-sensitized DSSCs from rational molecular engineering and electrolyte optimization

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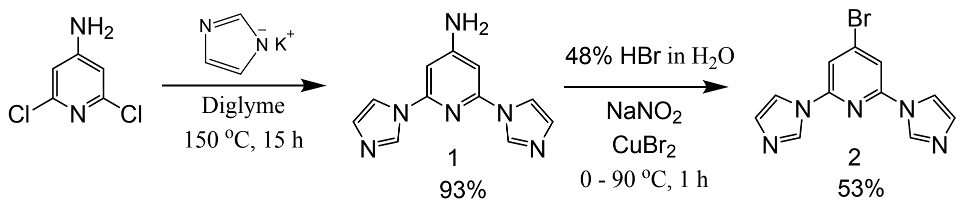
Synthesis of 2



Synthesis of *aminopyridine 1*

In a clean and dry 100 mL two-neck flask charged with imidazole (4.18 g, 61.35 mmol) and KOH (3.44 g, 61.35 mmol) flakes and heated at 250 °C under high vacuum and cooled to ambient temperature gave potassium salt of imidazole. Then added 4-amino-2,6-dichloropyridine (1.0 g, 6.13 mmol) in diglyme (20 mL) by vigorous stirring under Argon atmosphere at 150 °C for 18 h. The mixture was poured into water and the precipitate that formed was filtered and dried to isolate desired compound **1** (1.25 g, 93% yield). ^{1}H NMR (400 MHz, DMSO-d6, δ ppm): 8.43 (s, 2H), 7.78 (s, 2H), 7.02 (s, 2H), 6.62 (bs, 2H), 6.61 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d6, δ ppm): 159.6, 148.9, 135.65, 130.3, 117.0, 94.8. ESI-HRMS calcd for $C_{11}H_{11}N_6$ m/z = 227.1040. Found: 227.1038.

Synthesis of bromopyridine 2

To a solution of **1** (0.7 g, 3.09 mmol) in 15 mL HBr 48% in H_2O, a solution of $NaNO_2$ (0.213 g, 3.09 mmol) in 3.0 mL of H_2O was slowly added at 0 °C. The mixture was stirred for 15 min and added to a solution of $CuBr_2$ (0.345 g, 1.55 mmol) in 5.0 mL HBr 48%. The resulting mixture was stirred and refluxed for 1 h. The reaction mixture was quenched with 2N NaOH until pH ≈ 8. The suspension thus obtained was extracted with ethyl acetate (3 X 100 mL). The organic layer was washed with aqueous NaCl, dried over Na_2SO_4 and concentrated to dryness. The desired creamy colour compound 2 was obtained without purification and used directly for next step (0.48 g, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.36 (s, 2H), 7.62 (s, 2H), 7.44 (s, 2H), 7.24 (s, 2H). ^{13}C NMR (400 MHz, $CDCl_3$+CD3OD, δ ppm): 152.5, 141.3, 139.1, 134.4, 120.4, 117.4. ESI-HRMS calcd for $C_{11}H_9N_5Br$ m/z = 290.0036. Found: 290.0082.

Copies of NMR Spectra

Fig. S1: ^{1}H NMR spectrum of compound **1**.

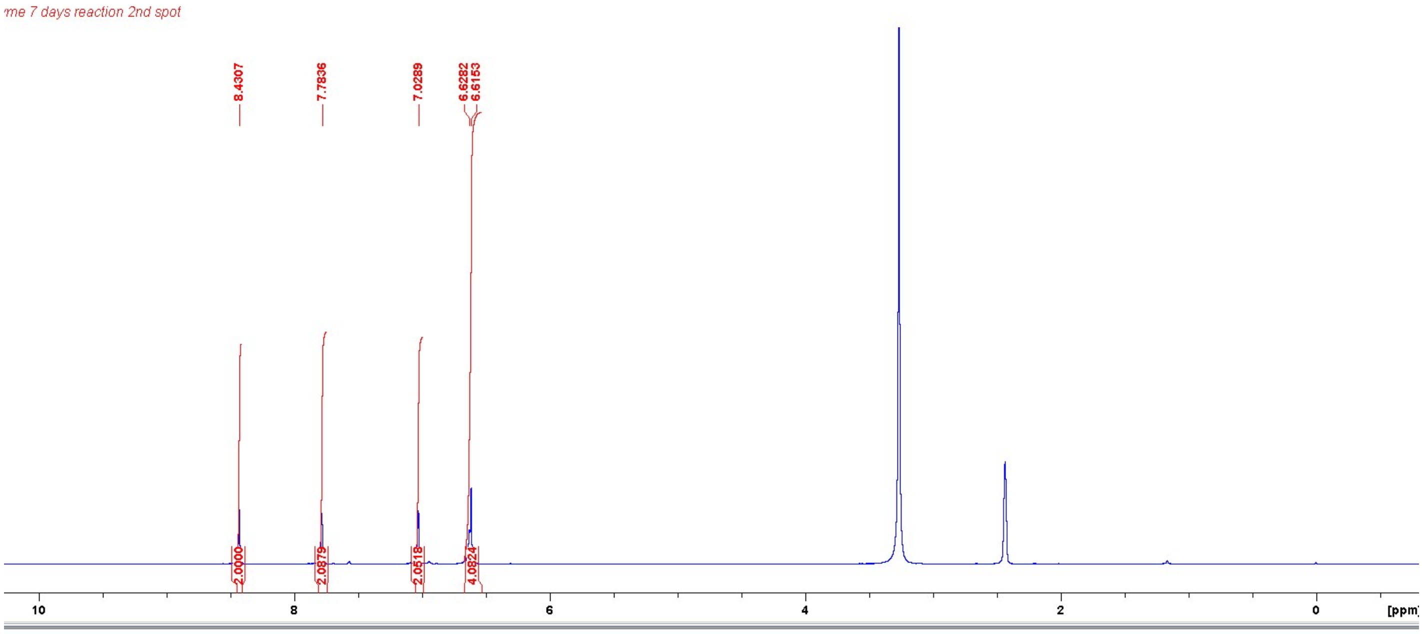


Fig. S2: ^{13}C NMR spectrum of compound **1**.

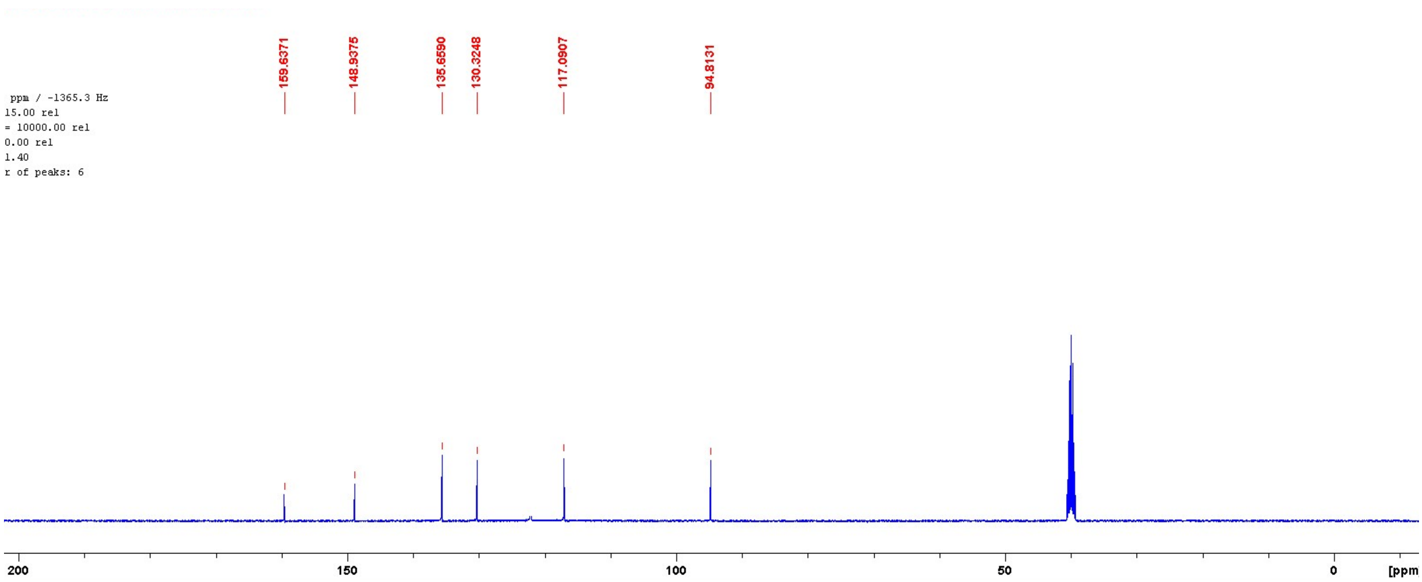


Fig. S3: ^{1}H NMR spectrum of compound **2**.

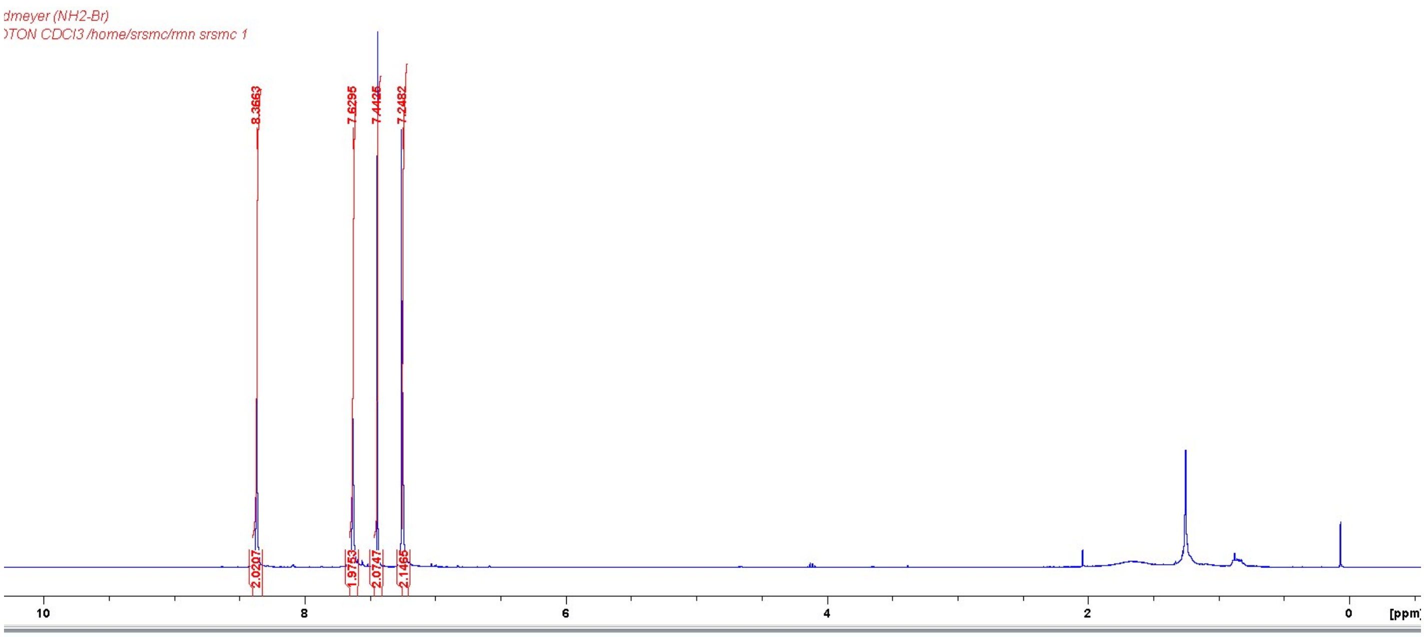


Fig. S4: ^{13}C NMR spectrum of compound **2**

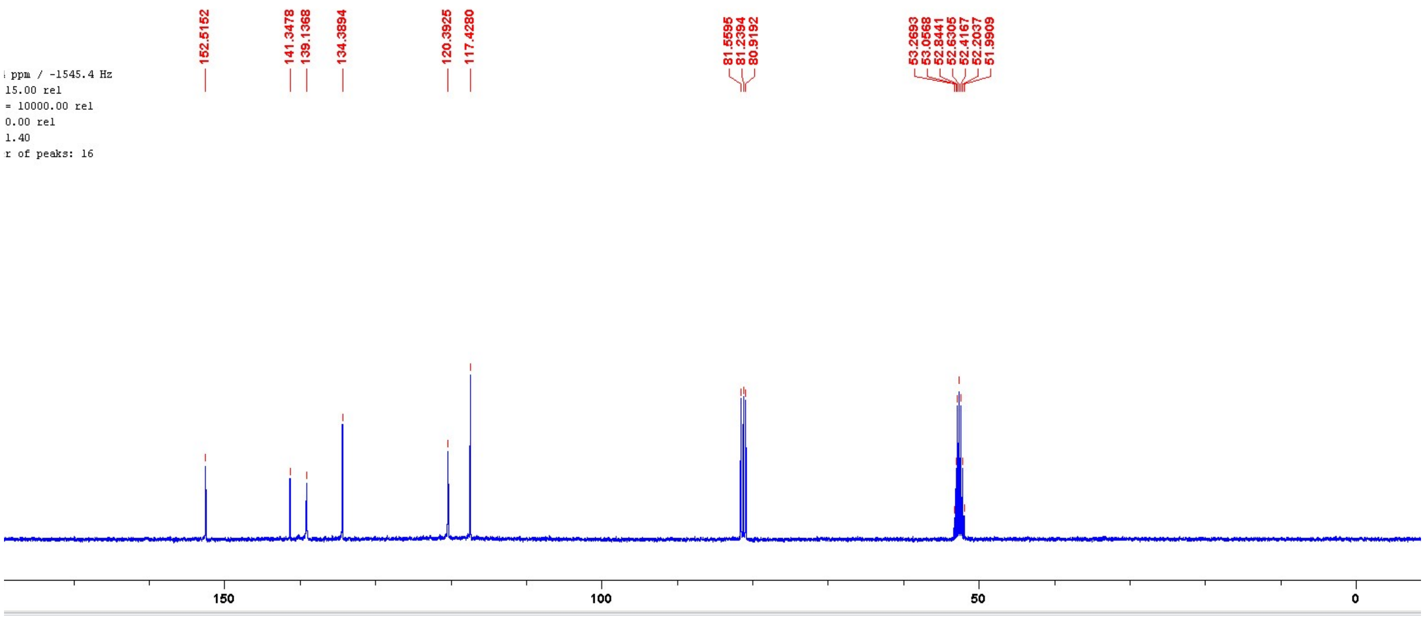


Fig. S5: ^{1}H NMR spectrum of compound **3**.

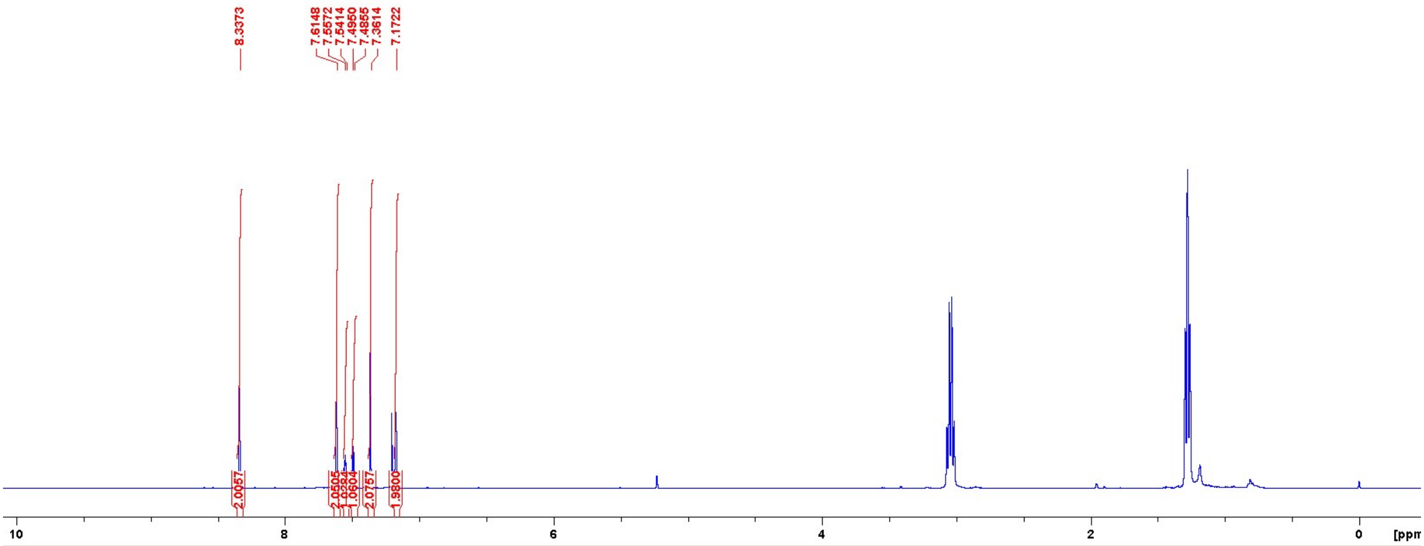


Fig. S6: ^{13}C NMR spectrum of compound **3**.

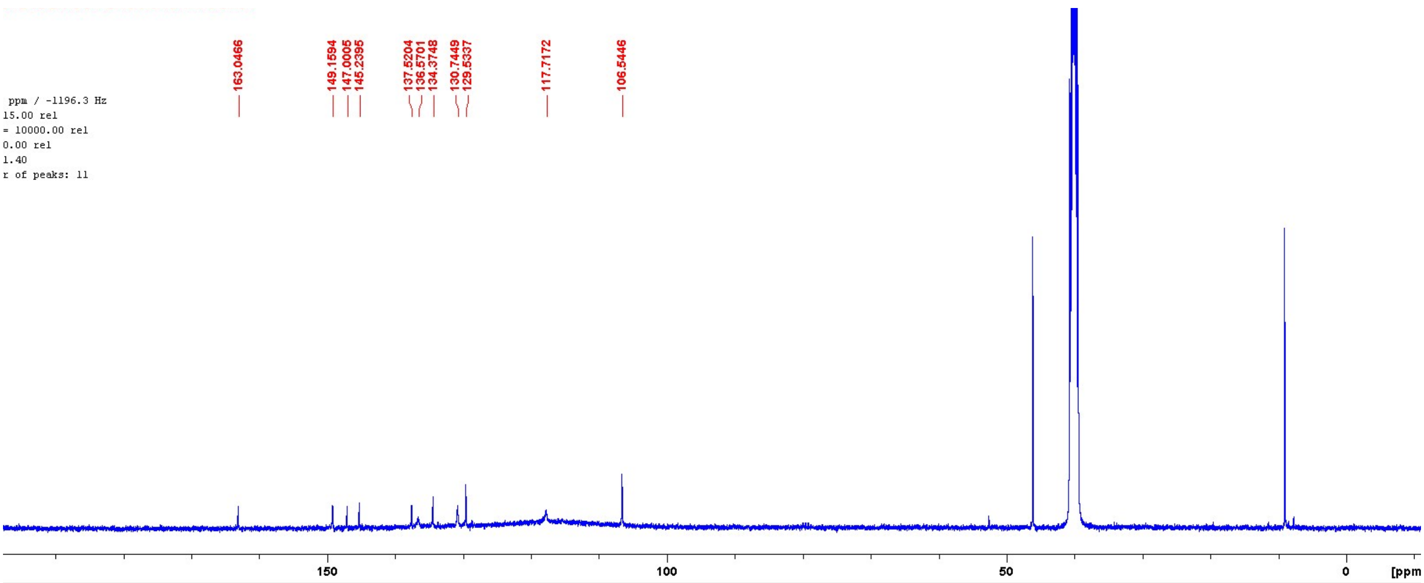


Fig. S7: [1]H NMR spectrum of **L2**.

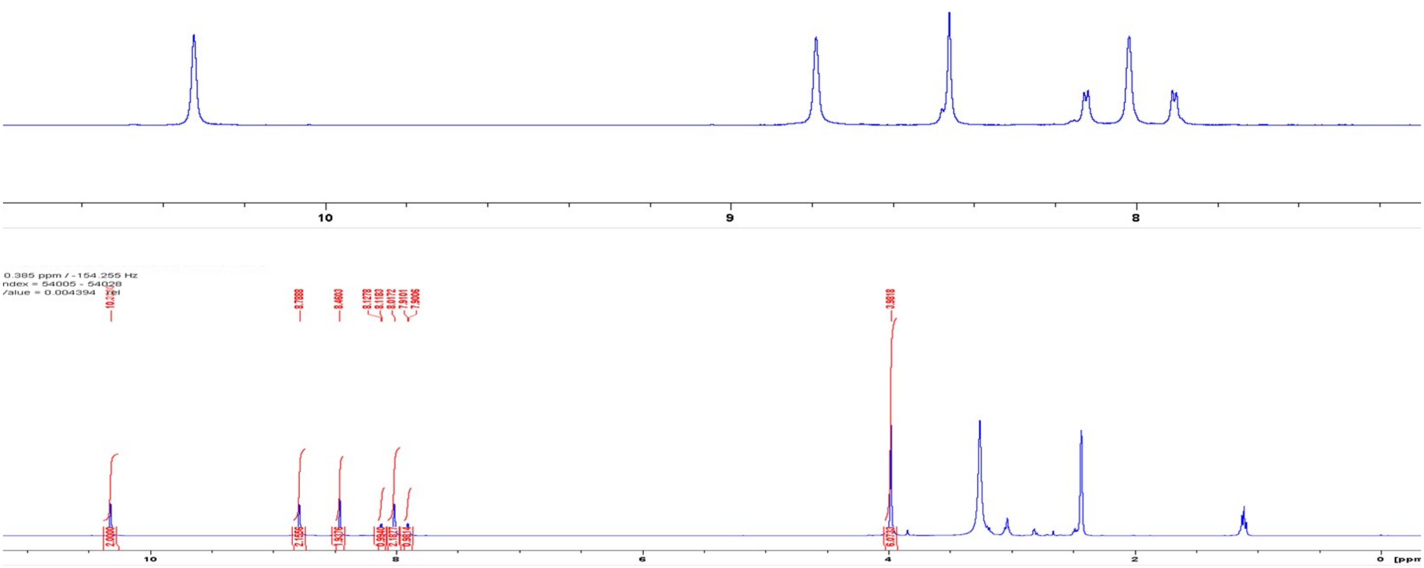
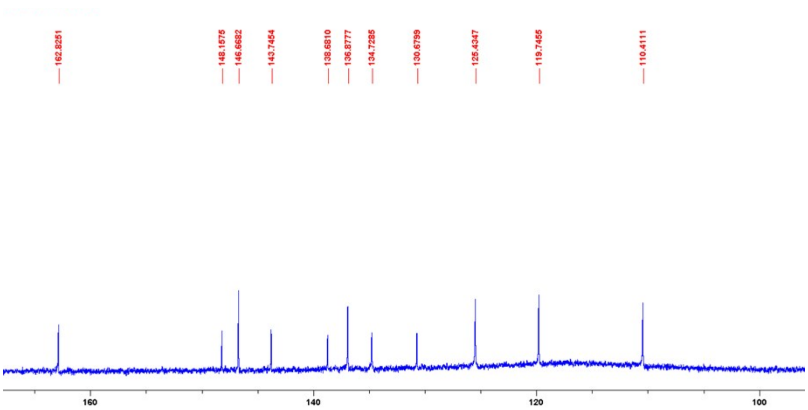


Fig. S8: [13]C NMR spectrum of **L2**.



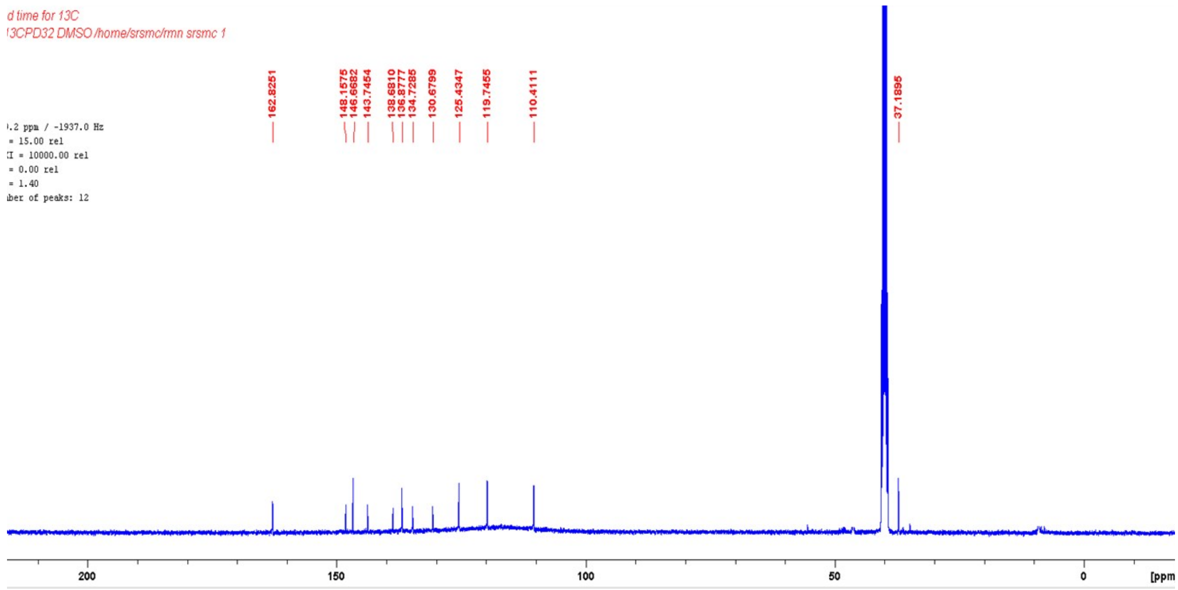


Fig. S9: [1]H NMR spectrum of compound 4.

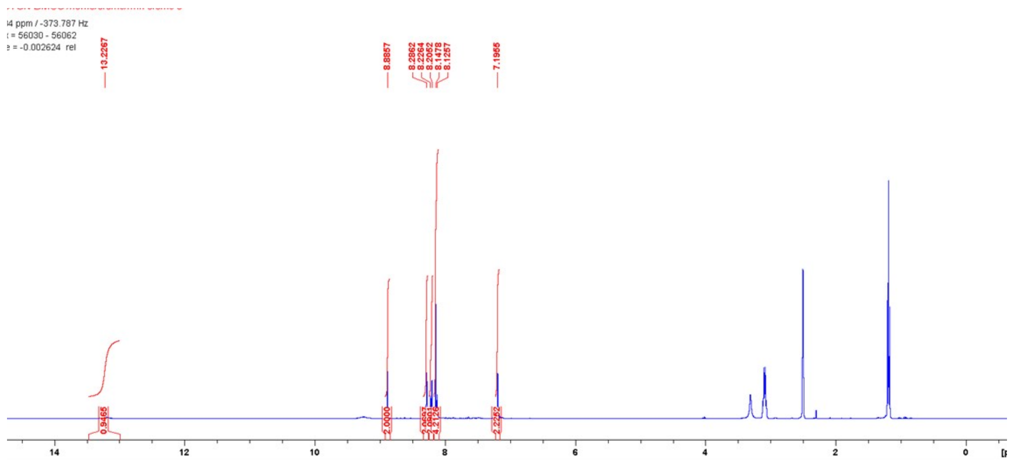


Fig. S10: [13]C NMR spectrum of compound 4.

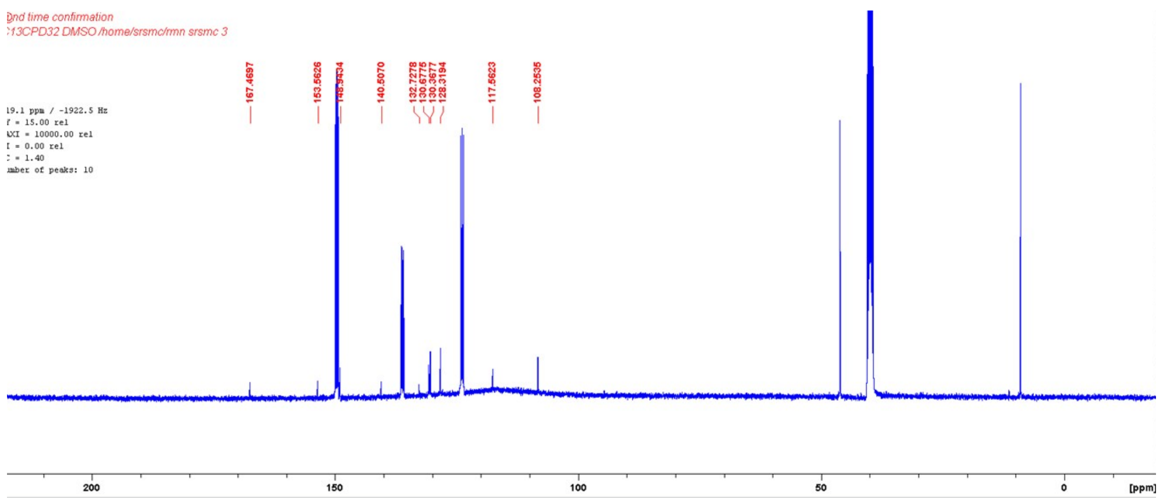


Fig. S11: ^{1}H NMR spectrum of L1.

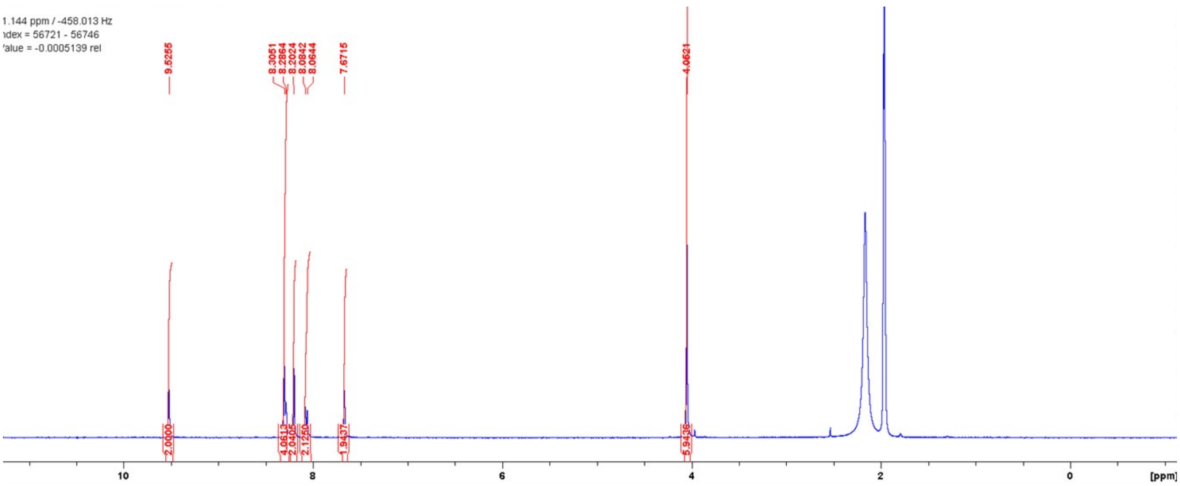


Fig. S12: ^{13}C NMR spectrum of L1.

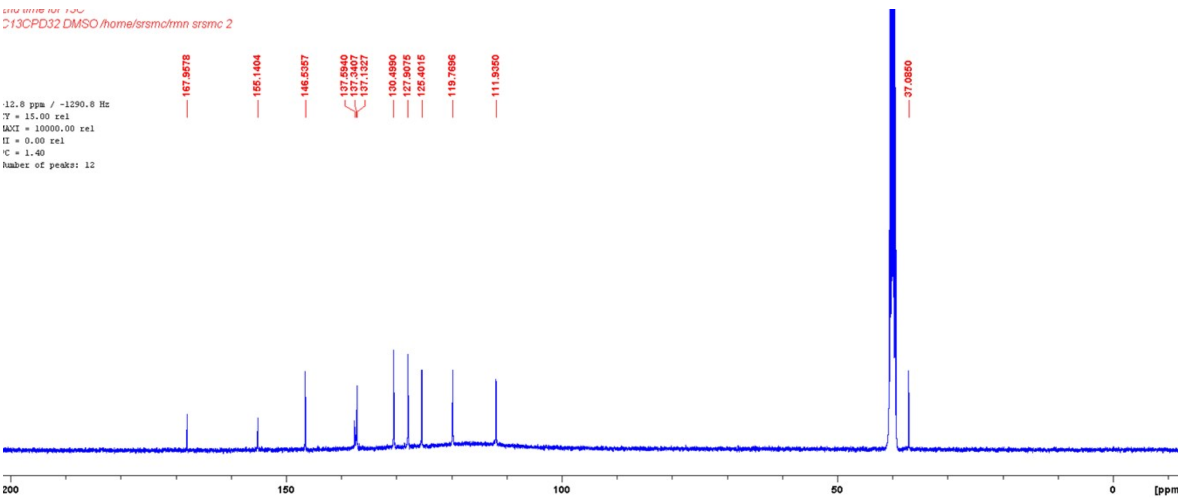
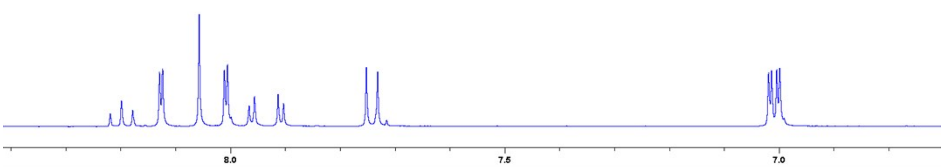


Fig. S13: ^{1}H NMR spectrum of ARM-7.



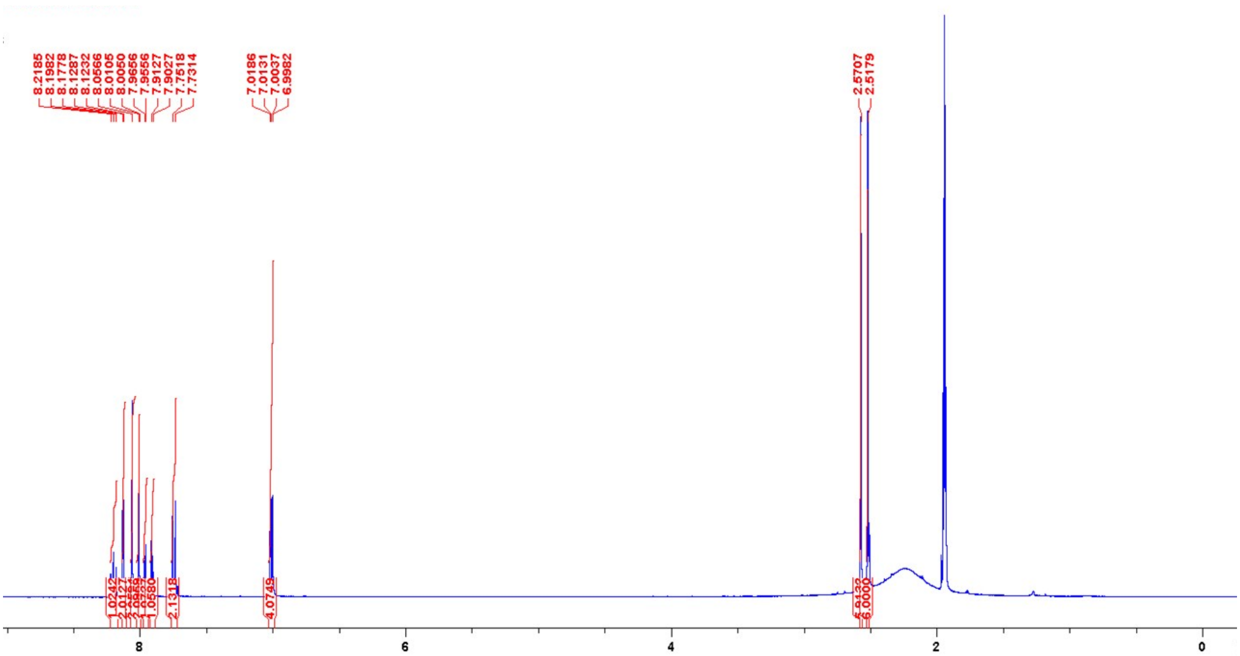


Fig. S14: ^{13}C NMR spectrum of ARM-7.

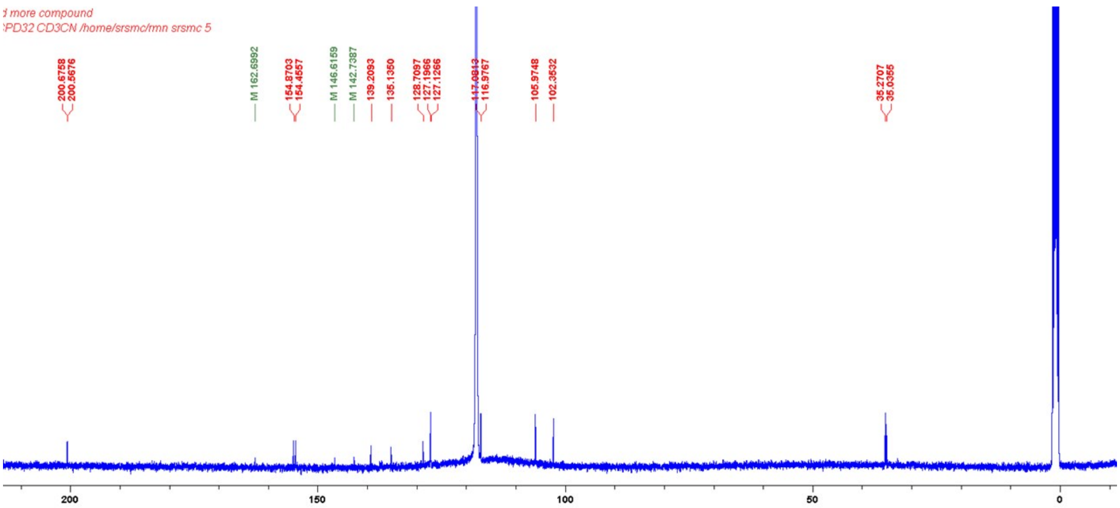
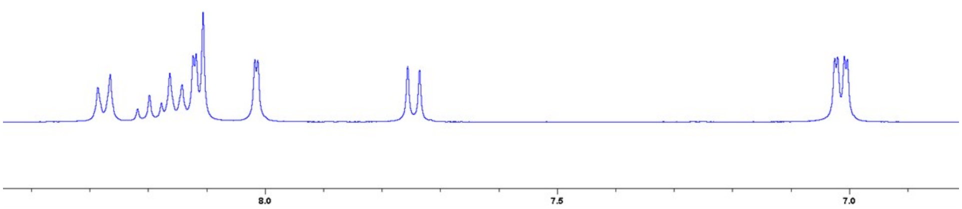


Fig. S15: ^{1}H NMR spectrum of ARM-11.



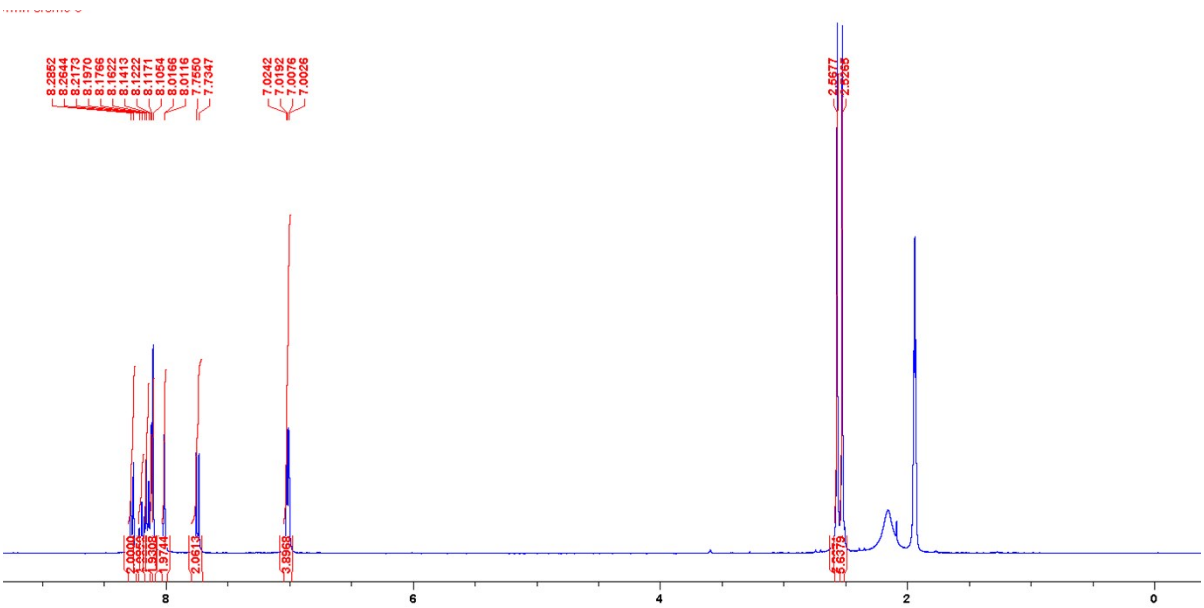
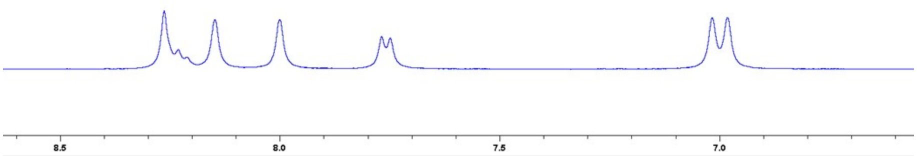
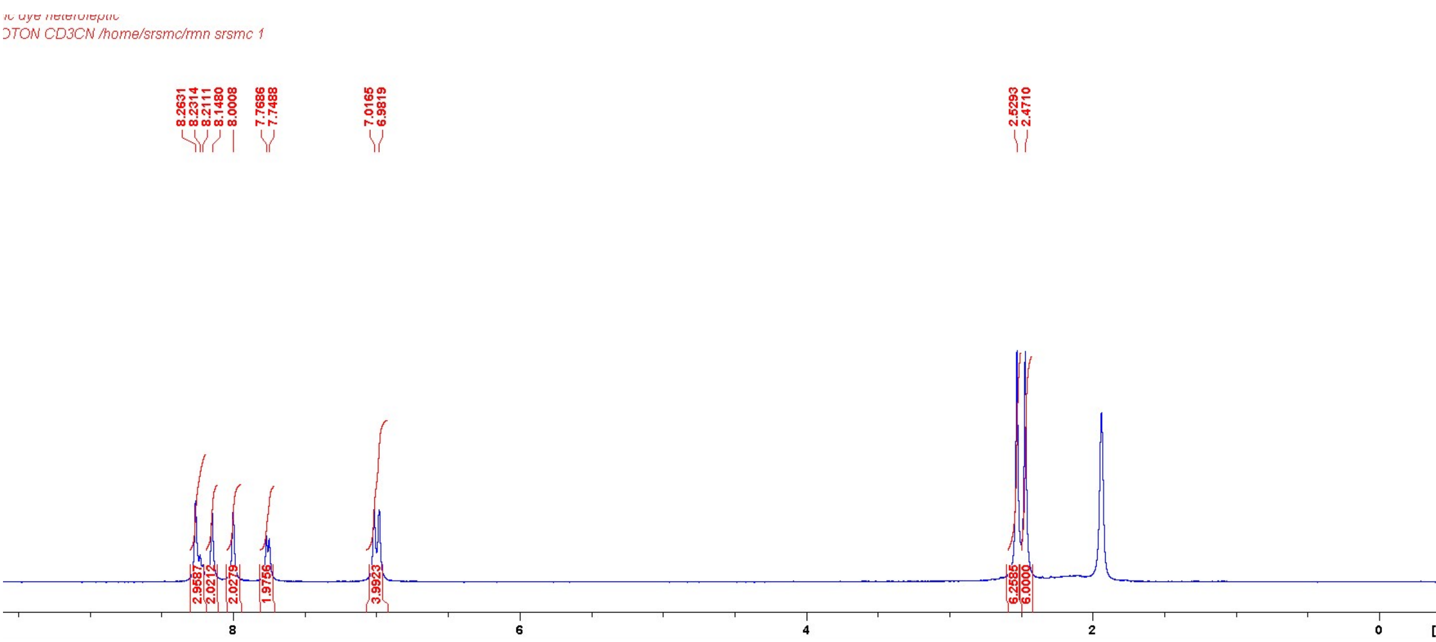


Fig. S16: ^{1}H NMR spectrum of ARM-13.





Computational details

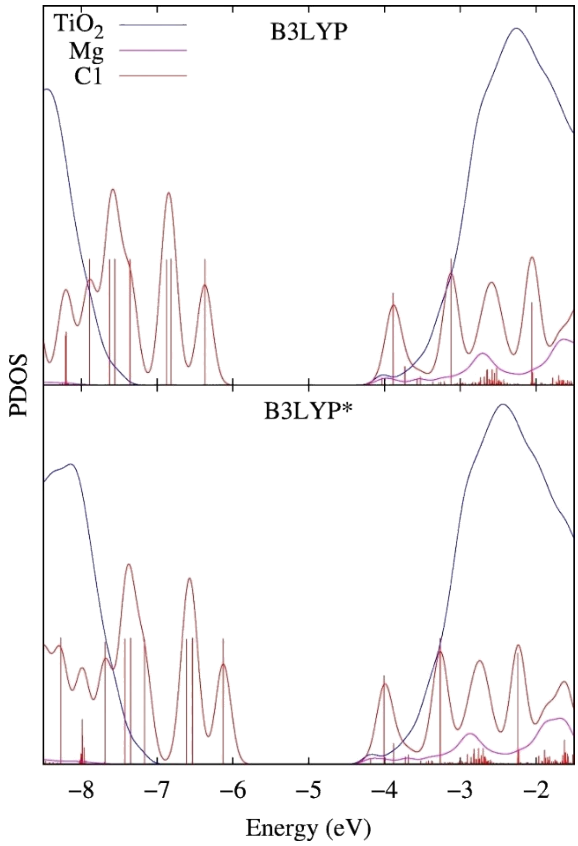


Figure S17. Projected Density of States (PDOS) of the C1@Mg-TiO_2 systems over the atoms belonging to the C1 dye (red), TiO_2 surface (blue) and Mg^{2+} cation (magenta) moieties as calculated by Mulliken population analysis and employing B3LYP (top) and B3LYP*(HF xc=15%, bottom panel) functionals. Note that for the sake of a better visualization, only the vertical bars conforming the C1 DOS are represented here and the TiO_2 DOS intensity has been divided by a factor of 10.

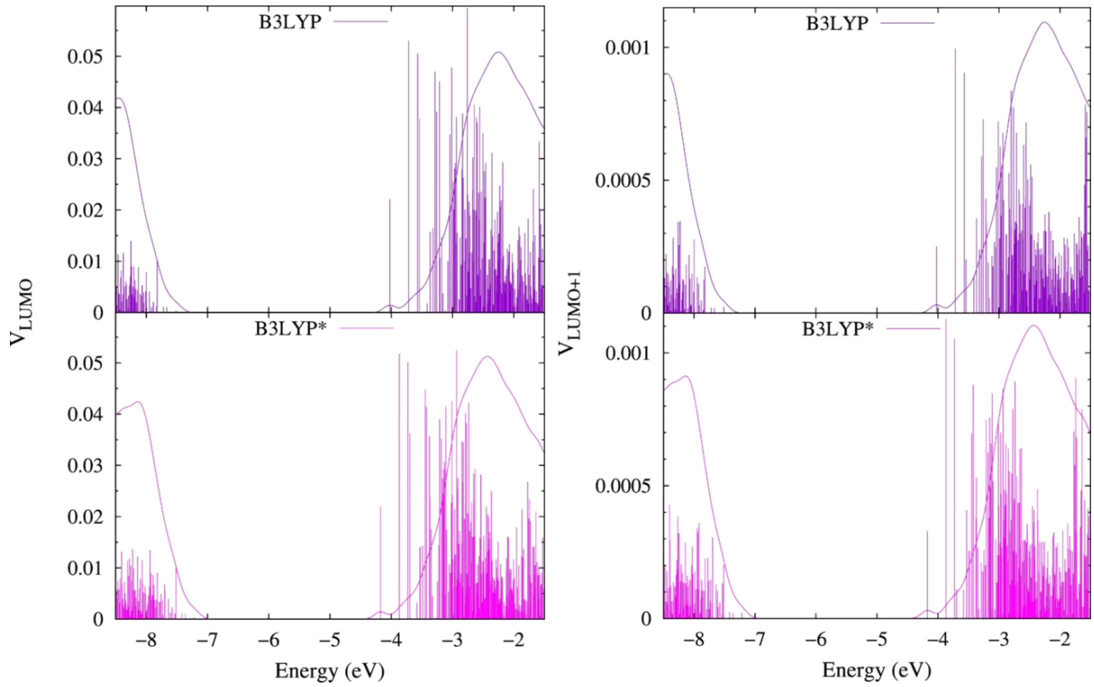


Figure S18. Electronic coupling V between the frontier unoccupied MOs of C1 and the states of the TiO2-Mg surface (vertical bars); and diabatic TiO_2-Mg DOS (continuous lines), as calculated by using B3LYP (purple) and B3LYP* (magenta color) functionals.

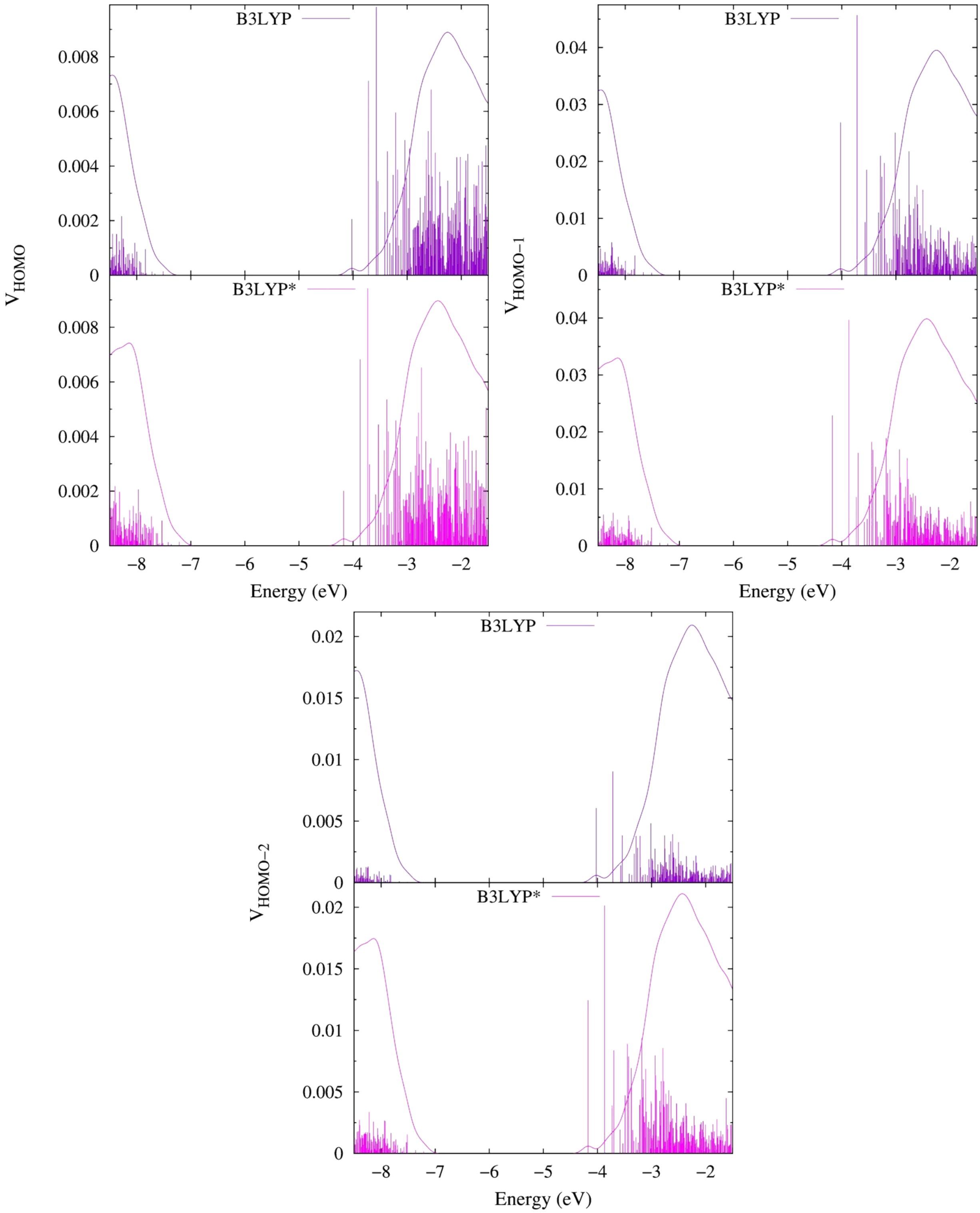


Figure S19 Electronic coupling *V* between the frontier occupied MOs of C1 and the states of the TiO2-Mg surface (vertical bars); and diabatic TiO_2-Mg DOS (continuous lines), as calculated by using B3LYP (purple) and B3LYP* (magenta color) functionals.

Table S1 Probability distributions (Γ) and related recombination/injection lifetimes (τ) calculated at the diabatic H-2, H-1, HOMO, LUMO and L+1 energies, as estimated by employing B3LYP and B3LYP* functionals. The relevant diabatic injection properties are marked with orange color.

Functional	Γ_{H-2} (eV)	Γ_{H-1} (eV)	Γ_{HOMO} (eV)	Γ_{LUMO} (eV)	Γ_{L+1} (eV)
B3LYP	3.32E-08	4.71E-07	1.56E-10	0.1640	5.36E-05
B3LYP*	1.83E-07	5.87E-07	3.40E-10	0.1673	7.54E-05
	τ_{H-2} (fs)	τ_{H-1} (fs)	τ_{HOMO} (fs)	τ_{LUMO} (fs)	τ_{L+1} (fs)
B3LYP	1.98E+07	1.40E+06	4.21E+09	4.01	12273
B3LYP*	3.61E+06	1.12E+06	1.93E+09	3.93	8723

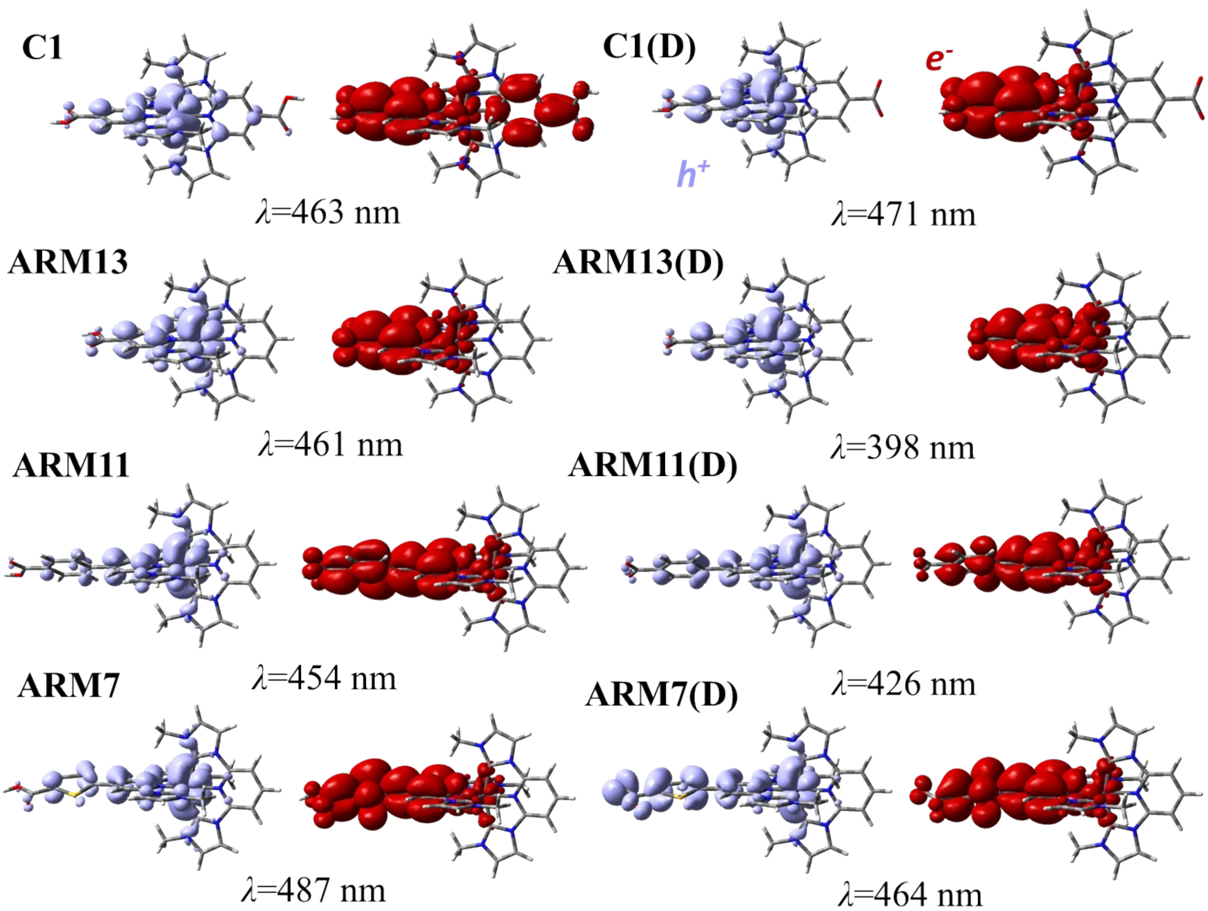


Figure S20. NTOs for the main transition forming the MLCT excitations of the Fe complex dyes studied in this work (C1, ARM13, ARM11 and ARM7 from top to the bottom) both in their protonated (left) and deprotonated (right) forms. Purple/red colors are employed to display hole/electron isodensity plots. The isovalues used for this plot was 0.02 a.u.

Table S2 State Number (*n*), excitation energies (E_x), wavelengths (λ), oscillator strengths (f), major contributions and related percentage (%) of the main transitions in the visible region for the protonated dyes C1, ARM13, ARM11 and ARM7. Transitions related with MLCT excitations are marked with orange color.

	n	E_x (eV)	*λ* (nm)	*f* (a.u.)	*Transition*	%
C1	1	2.1	591	0	H→ L	66.6
	5	2.68	463	0.308	H-2→ L+1	45.4
	9	3.23	384	0.155	H→ L+3	69.4
ARM13	1	2.04	607	0	H→L	70
	4	2.69	461	0.148	H-2→ L	63.4
	9	3.22	385	0.15	H→ L+3	55
ARM11	1	2.23	555	0	H→L	69.1
	4	2.73	454	0.271	H-1→ L	64.4
	9	3.2	388	0.209	H-2→ L+1	58.8
ARM7	1	2.04	607	0	H→L	69.5
	3	2.54	487	0.371	H-1→ L	67.1
	9	3.17	391	0.135	H→ L+3	50.2

Table S3 Experimental and calculated ground/excited state oxidation potentials (GSOPs/ESOPs) in eV versus SCE of C1, ARM7, ARM11 and ARM13.

	Experiments		*Theory*	
Dye	GSOP	ESOP (GSOP-E_{0-0})	GSOP	ESOP (GSOP-E_{max})
C1	0.85	-1.40	1.08	-1.60
ARM13	0.82	-1.47	1.00	-1.69
ARM11	0.70	-1.65	0.92	-1.81
ARM7	0.74	-1.51	0.93	-1.61

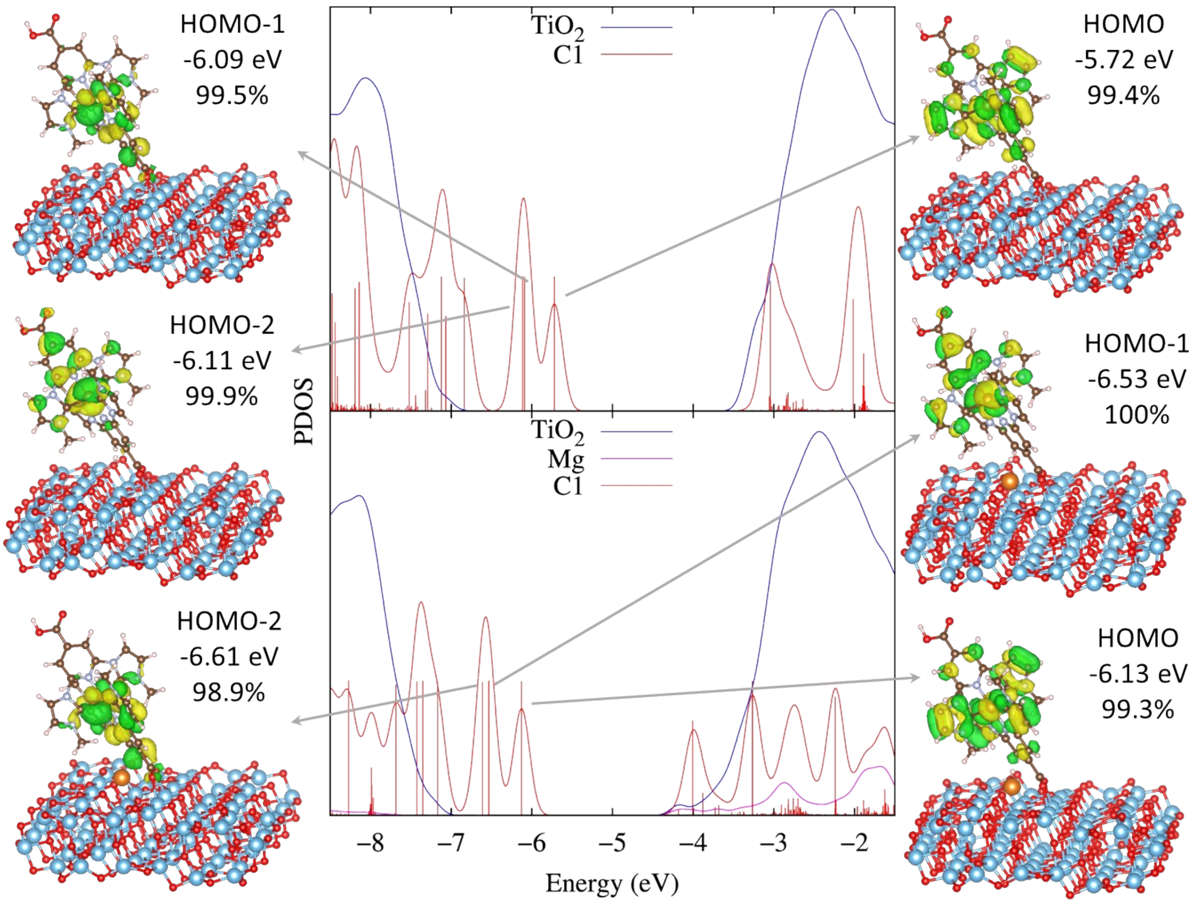


Figure S21 Projected Density of States (PDOS) of the C1@TiO_2 (top) and C1@Mg-TiO_2 (bottom panel) systems over the atoms belonging to the C1 dye (red), TiO_2 surface (blue) and Mg^{2+} cation (magenta) moieties as calculated by Mulliken population analysis. Note that for the sake of a better visualization, only the vertical bars conforming the C1 DOS are represented here and the TiO_2 DOS intensity has been divided by a factor of 10. The isodensity plots of the relevant dye occupied MOs indicated by the grey arrows are displayed in the onsets of the PDOS plot. The energies and weight percentages for each plotted MOs are reported as well. The isovalue used in the isodensity plots was 0.02 a.u.

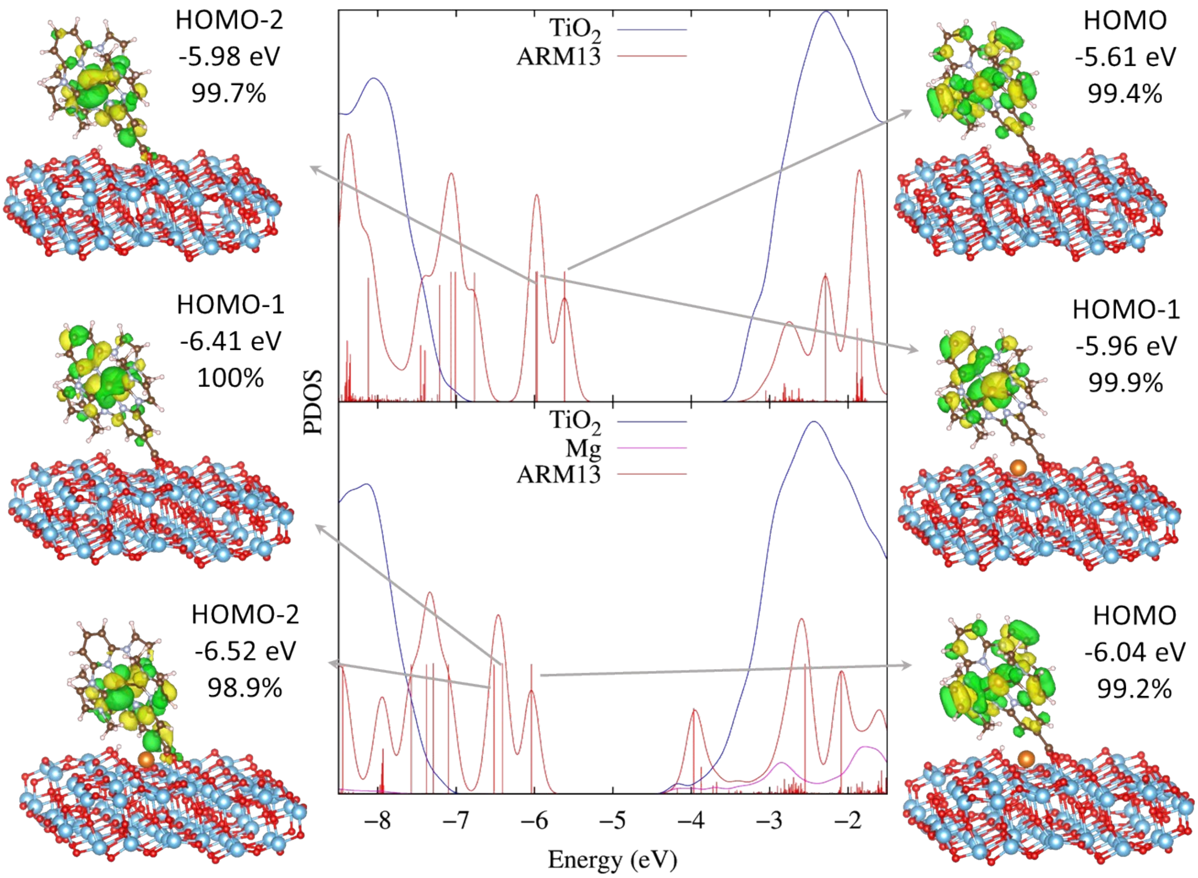


Figure S22 Projected Density of States (PDOS) of the ARM13@TiO_2 (top) and ARM13@Mg-TiO_2 (bottom panel) systems over the atoms belonging to the ARM13 dye (red), TiO_2 surface (blue) and Mg^{2+} cation (magenta) moieties as calculated by Mulliken population analysis. Note that for the sake of a better visualization, only the vertical bars conforming the ARM13 DOS are represented here and the TiO_2 DOS intensity has been divided by a factor of 10. The isodensity plots of the relevant dye occupied MOs indicated by the grey arrows are displayed in the onsets of the PDOS plot. The energies and weight percentages for each plotted MOs are reported as well. The isovalue used in the isodensity plots was 0.02 a.u.

Table S4 Diabatic energy levels for the dye (H-2, H-1, HOMO, LUMO and L+1 energies) and TiO_2 surface (Conductance Band Minimum (CBM) and Valence Band Minimum (VBM)) with their corresponding energy gaps (E_g), for C1@TiO_2, C1@Mg-TiO_2, ARM13@TiO_2 and ARM13@Mg-TiO_2 systems. All values are given in eV.

Dye@ TiO_2	H-2	H-1	HOMO	LUMO	L+1	E_g@Dye	VBM	CBM	E_g@TiO_2
C1	-6.11	-6.08	-5.72	-3.04	-2.66	2.66	-7.07	-3.34	3.72
C1-Mg	-6.54	-6.52	-6.11	-3.38	-3.26	2.74	-7.21	-4.17	3.04
ARM13	-5.98	-5.96	-5.61	-2.6	-2.29	3.01	-7.05	-3.34	3.71
ARM13-Mg	-6.43	-6.41	-6.02	-3.34	-2.55	2.69	-7.21	-4.17	3.05

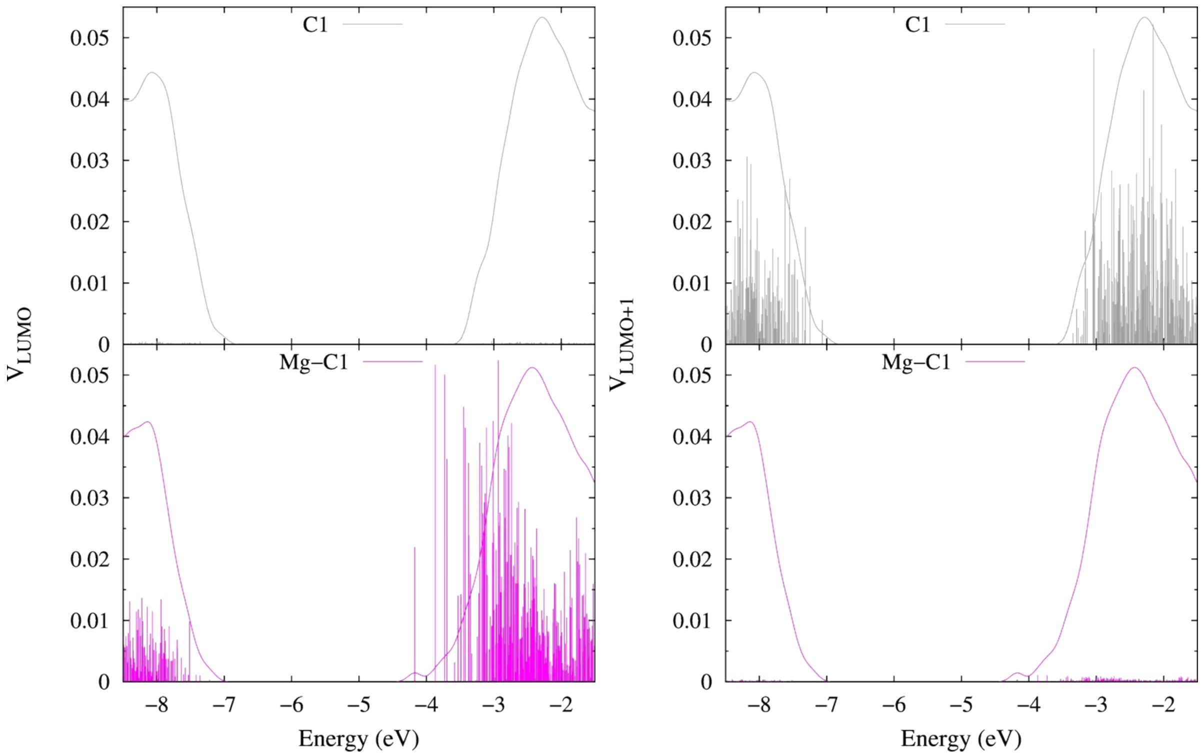


Figure S23 Calculated electronic coupling *V* between the frontier unoccupied MOs of C1 and the states of the TiO_2 (grey) and TiO_2-Mg (magenta color) surfaces (vertical bars); the corresponding diabatic TiO_2 and TiO_2-Mg DOS (dashed lines) are also reported.

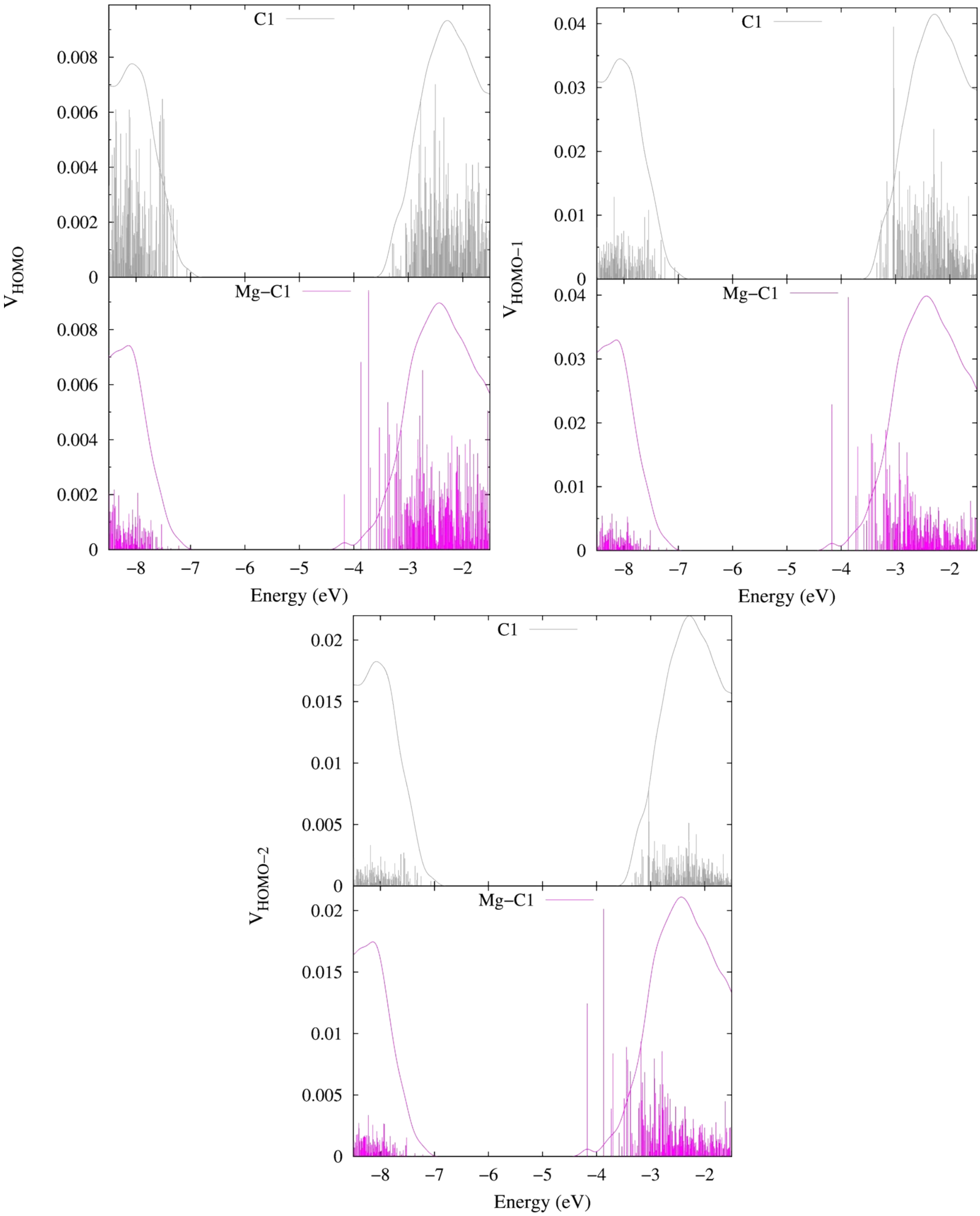


Figure S24 Calculated electronic coupling *V* between the frontier occupied MOs of C1 and the states of the TiO_2 (grey) and TiO_2-Mg (magenta color) surfaces (vertical bars); the corresponding diabatic TiO_2 and TiO_2-Mg DOS (dashed lines) are also reported.

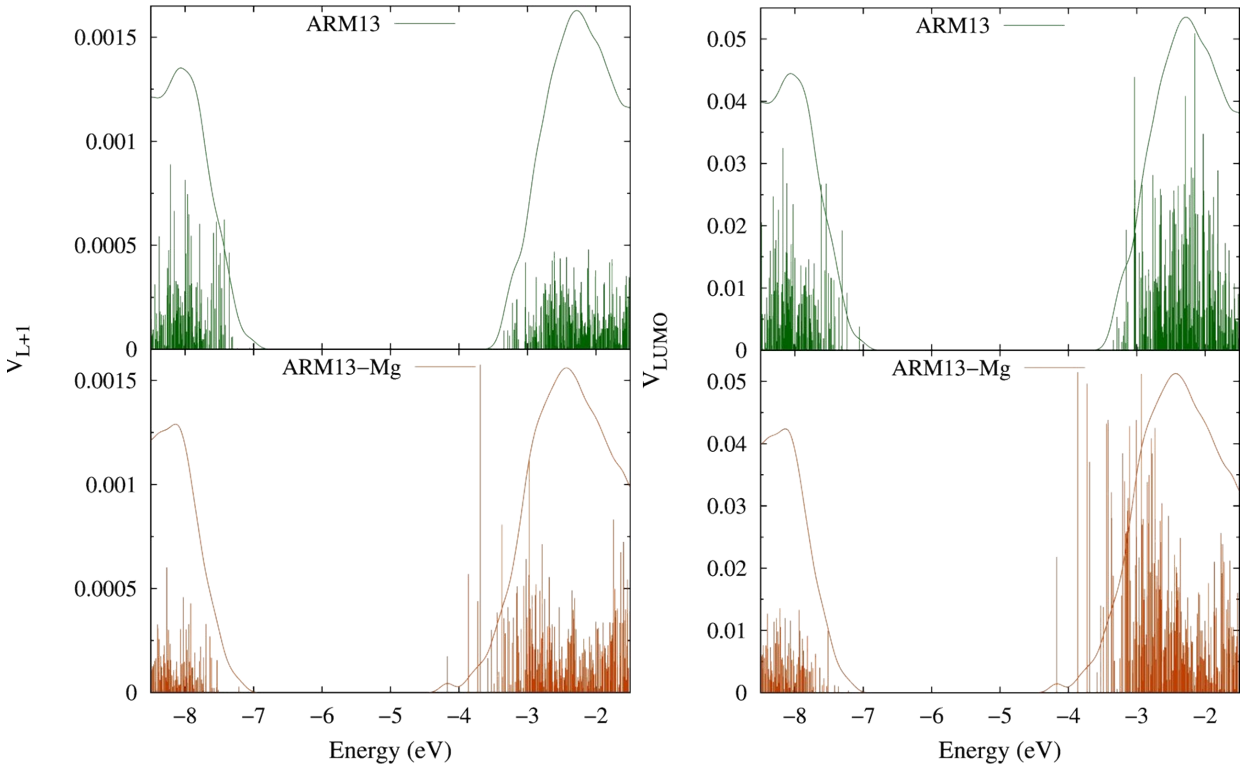


Figure S25 Calculated electronic coupling *V* between the frontier unoccupied MOs of ARM13 and the states of the TiO_2 (grey) and TiO_2-Mg (magenta color) surfaces (vertical bars); the corresponding diabatic TiO_2 and TiO_2-Mg DOS (dashed lines) are also reported.

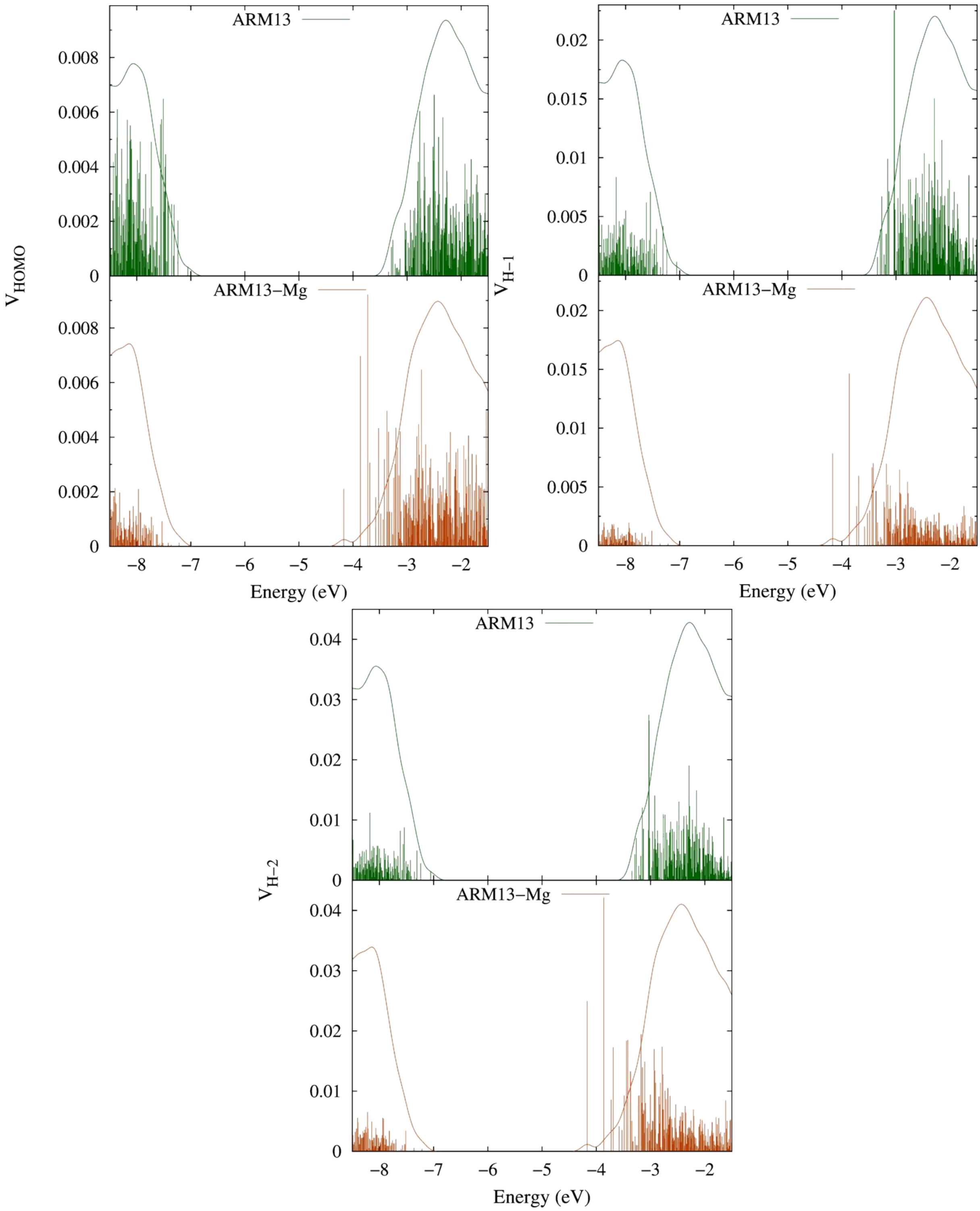


Figure S26. Calculated electronic coupling *V* between the frontier occupied MOs of ARM13 and the states of the TiO_2 (grey) and TiO_2-Mg (magenta color) surfaces (vertical bars); the corresponding diabatic TiO_2 and TiO_2-Mg DOS (dashed lines) are also reported.

Table S5 Probability distributions (Γ) and related recombination/injection lifetimes (τ) calculated at the diabatic H-2, H-1, HOMO, LUMO and L+1 energies for C1@TiO_2, C1@Mg-TiO_2, ARM13@TiO_2 and ARM13@Mg-TiO_2. The relevant diabatic injection properties are marked with orange color.

Dye@TiO_2	Γ_{H-2} (eV)	Γ_{H-1} (eV)	Γ_{HOMO} (eV)	Γ_{LUMO} (eV)	Γ_{L+1} (eV)
C1	2.28E-08	2.83E-07	2.18E-10	1.12E-05	0.142
C1-Mg	1.83E-07	5.87E-07	3.40E-10	0.167	7.54E-05
ARM13	4.93E-08	2.62E-08	4.13E-11	0.152	3.07E-05
ARM13-Mg	2.49E-07	2.72E-08	9.13E-11	0.179	4.43E-05
	τ_{H-2} (fs)	τ_{H-1} (fs)	τ_{HOMO} (fs)	τ_{LUMO} (fs)	τ_{L+1} (fs)
C1	2.89E+07	2.32E+06	3.01E+09	58530	4.63
C1-Mg	3.61E+06	1.12E+06	1.93E+09	3.93	8723
ARM13	1.33E+07	2.51E+07	1.59E+10	4.33	21428
ARM13-Mg	2.64E+06	2.42E+07	7.20E+09	3.67	14840

Cyclic Voltammetry of sensitized thin films

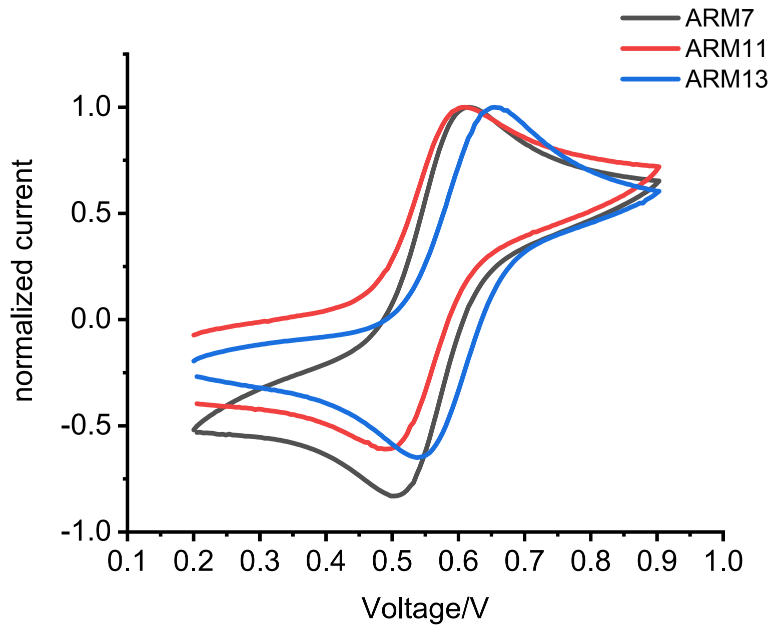


Figure S27. Normalized cyclic voltammetry recorded on TiO_2 for ARM7, ARM11 and ARM13 (black, red, and blue line respectively). The voltage is referred to double jacket SCE

Characterization of Photoanodes

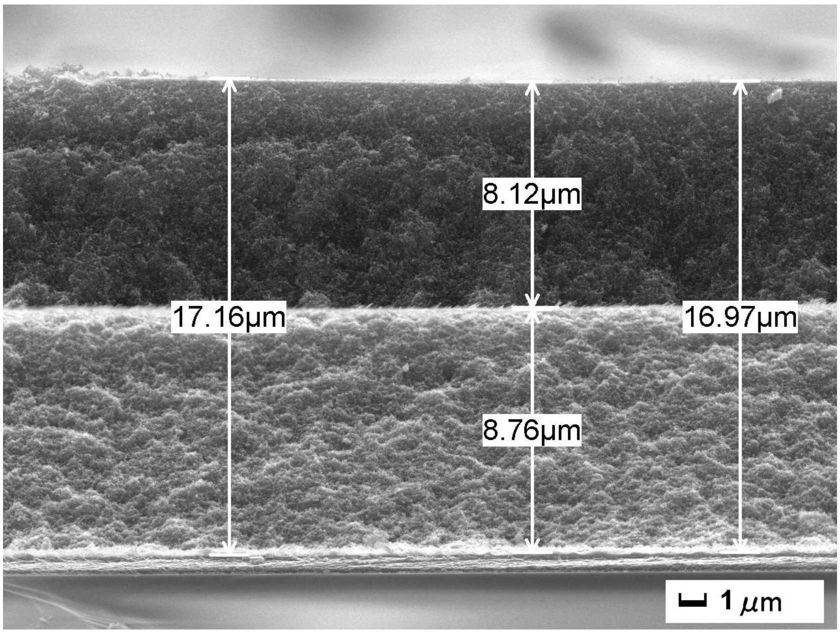


Figure S28 SEM cross-section of a two-layered TiO_2 electrode. Each 18 NRT anatase film accounts for a thickness of ca. 8.5 microns

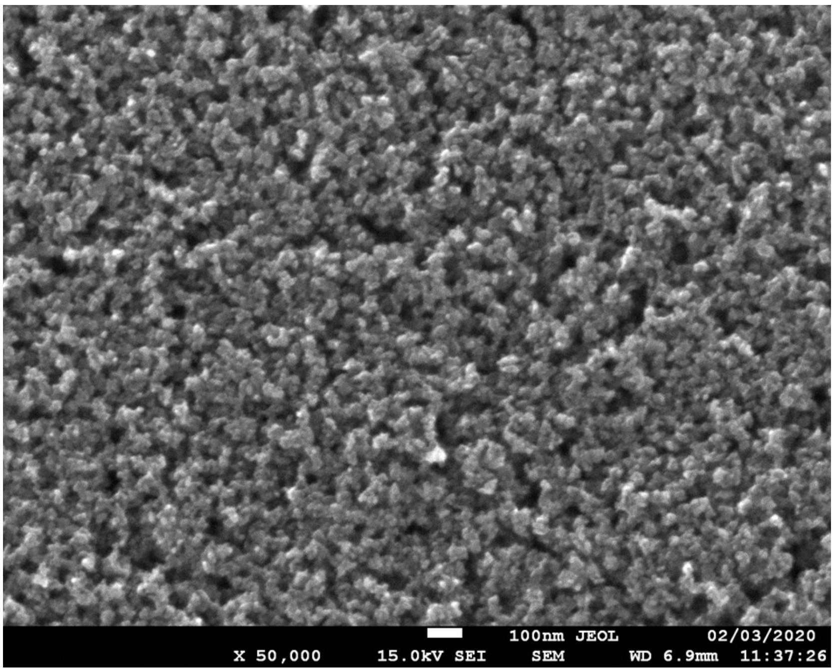


Figure S29 SEM top view showing the nanocrystalline nature of 18NRT TiO_2 electrodes annealed at 500 °C

Steady State and Transient Absorption Spectroscopy of sensitized thin films

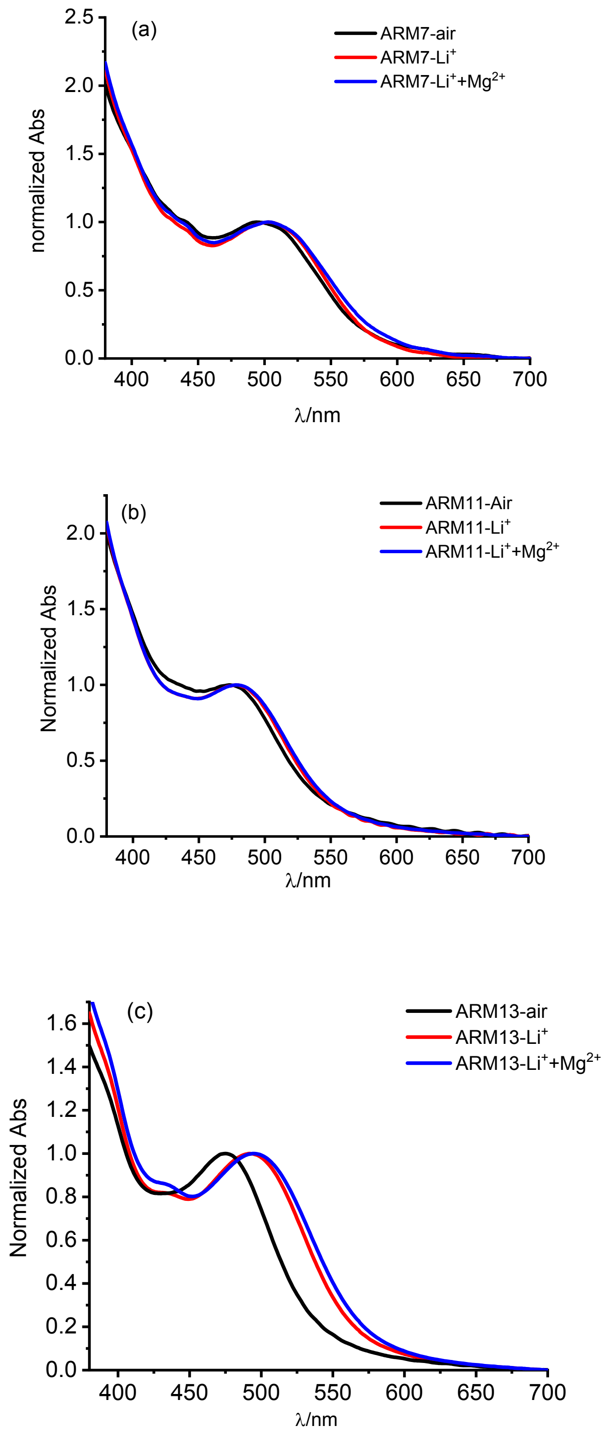


Figure S30 Shift of the absorption spectra of the Fe(II)NHC series for ARM7 (a), ARM11 (b) and ARM13 (c) in contact with air, Li^+ electrolyte (0.6 M PMIOTf + 0.1 M LiOTf + 0.1 M GuNCS + 0.1 M $TBAPF_6$ in acetonitrile) and Li^+ + Mg^{2+} electrolyte (0.6 M PMIOTf + 0.1 M LiOTf + 0.1 M GuNCS + 0.1 M $TBAPF_6$ + 0.1 M MgOTf in acetonitrile)

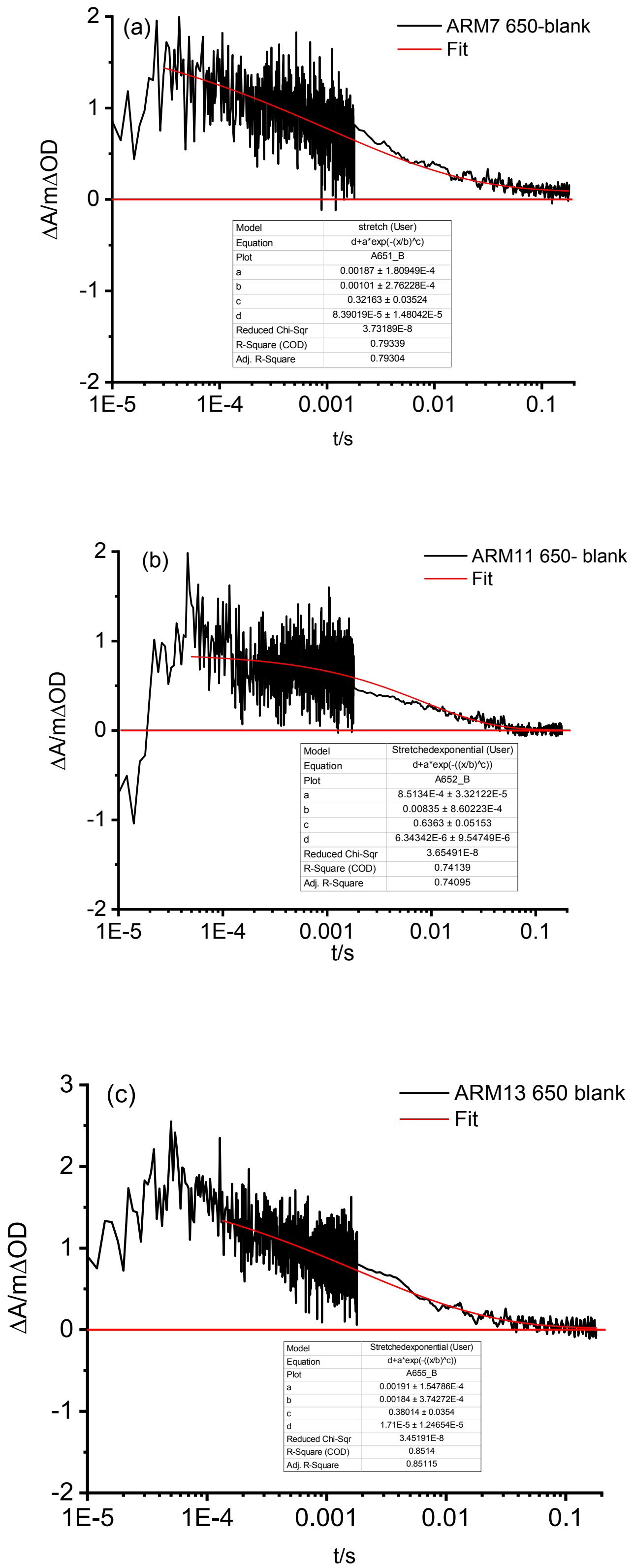
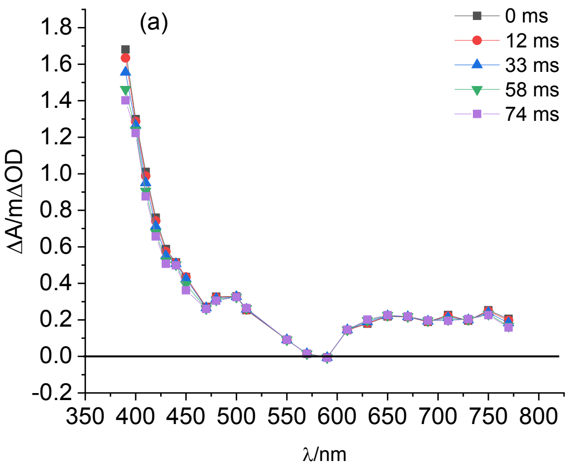
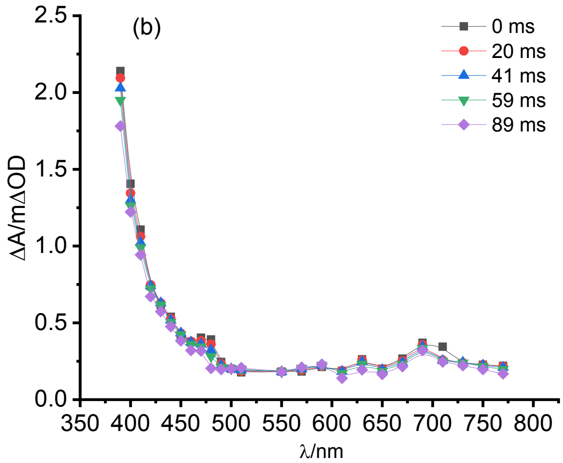


Figure S31 µs-s recombination kinetics observed at 650 nm in the presence of blank *electrolyte 3* (0.6 M PMIOTf + 0.1 M LiOTf + 0.1 M GuNCS + 0.1 M MgOTf + 0.1 M $TBAPF_6$ in acetonitrile) for ARM7(a), ARM11(b) and ARM13(c)





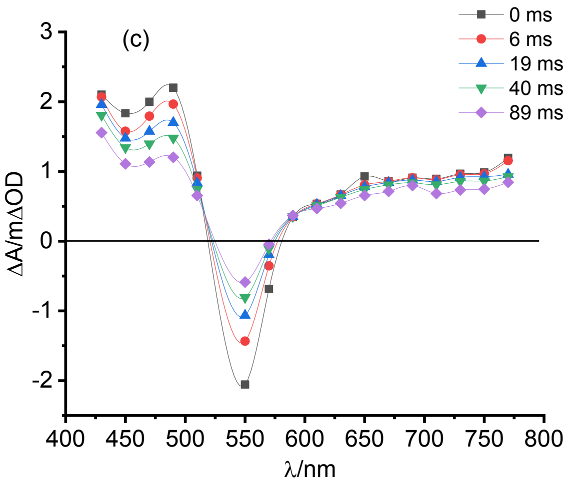


Figure S32 ms-time scale TAS (1 MOhm input impedance) of Fe(II)NHC sensitized films for ARM7 (a), ARM11 (b) and C1 (c) in contact with *electrolyte 3* deprived of I_2. All the spectra are characterized by general features like absorption of I_2 generated upon Fe(II) regeneration at 420 nm, stark absorption at 500 nm, bathochromic shifted bleach and absorption of electrons in TiO_2 trap states starting from 600 nm

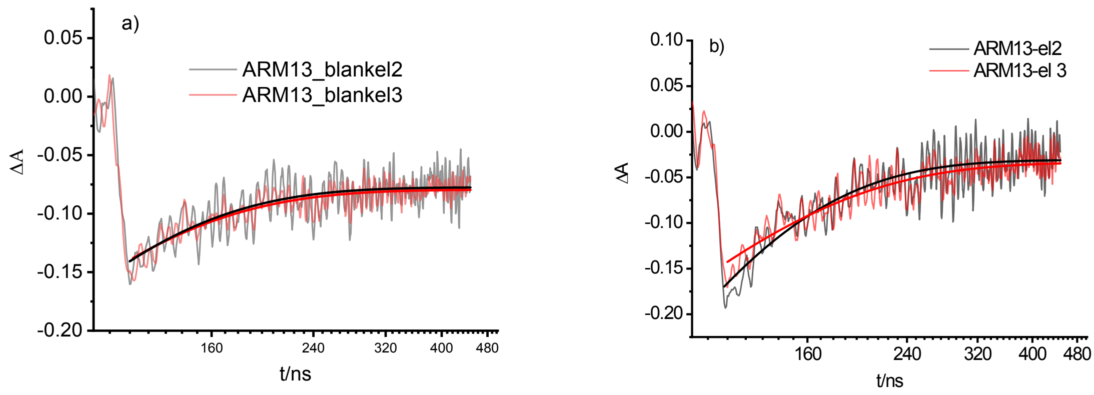


Figure S33 (a), Recombination dynamics recorded at 500 nm for ARM13 dyed film in contact with blank *electrolyte 2* (0.6 M PMIOTf + 0.1 M LiOTf + 0.1 M GuNCS + 0.1 M $MgOTF_2$ in acetonitrile) and blank *electrolyte 3* (0.6 M PMIOTf + 0.1 M LiOTf + 0.1 M GuNCS + 0.1 $MgOTf_2$ + 0.1 M $TBAPF_6$in acetonitrile). (b), Regeneration dynamics of ARM13 in presence of the reduced form of *electrolyte 2* (0.6 M PMII + 0.1 M LiI + 0.1 M GuNCS + 0.1 M MgI_2 in acetonitrile) and *3* (0.6 M PMII + 0.1 M LiI + 0.1 M GuNCS + 0.1 M MgI_2 + 0.1 M TBAI in acetonitrile)

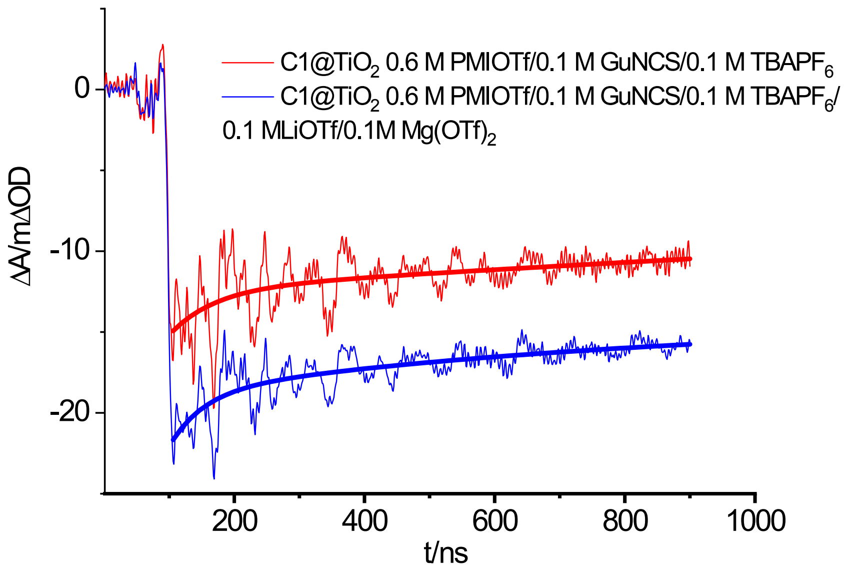


Figure S34 500 nm kinetics for **C1** dyed film in contact with 0.6 M PMIOTf + 0.1 M GuNCS + 0.1 M $TBAPF_6$ and with 0.6 M PMIOTf + 0.1 M GuNCS + 0.1 M $TBAPF_6$ + 0.1 M LiOTf + 0.1 M $Mg(OTf)_2$

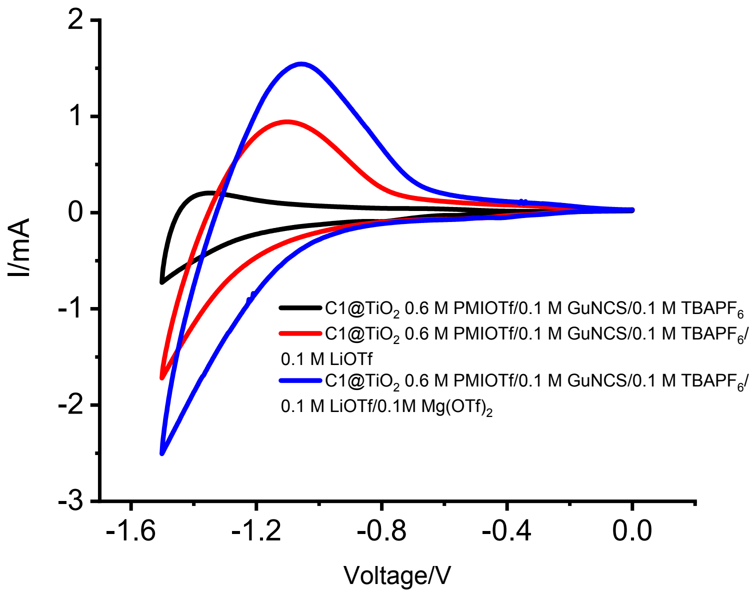


Figure S35 Cyclic voltammetry of **C1** dyed film in contact with 0.6 M PMIOTf + 0.1 M GuNCS + 0.1 M $TBAPF_6$, with 0.6 M PMIOTf + 0.1 M GuNCS + 0.1 M $TBAPF_6$ + 0.1 M LiOTf and with 0.6 M PMIOTf + 0.1 M GuNCS + 0.1 M $TBAPF_6$ + 0.1 M LiOTf + 0.1 M $Mg(OTf)_2$

Photovoltaic properties

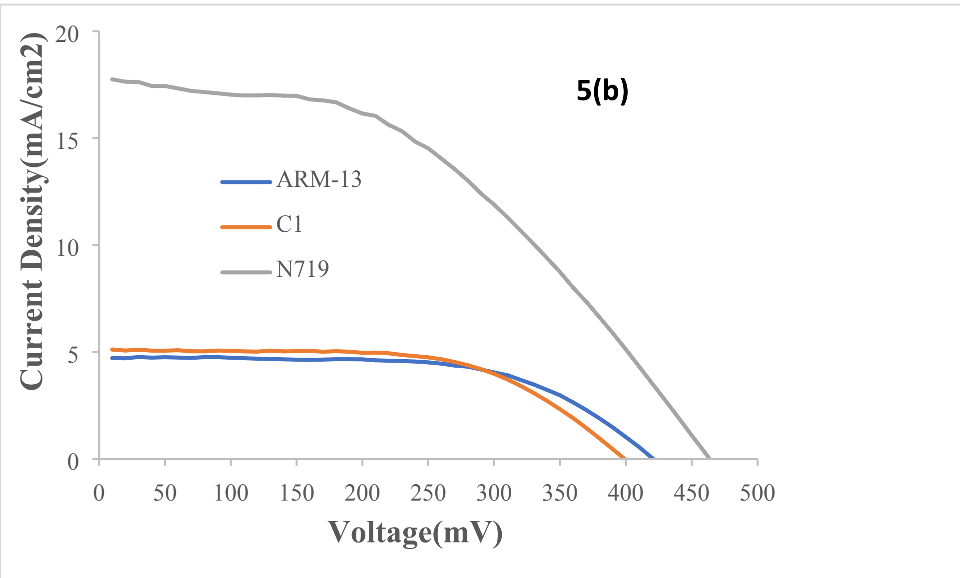


Figure S36 JV curves of the N719, ARM13 and C1 in the presence of *electrolyte 2* in ACN with the scattering layer

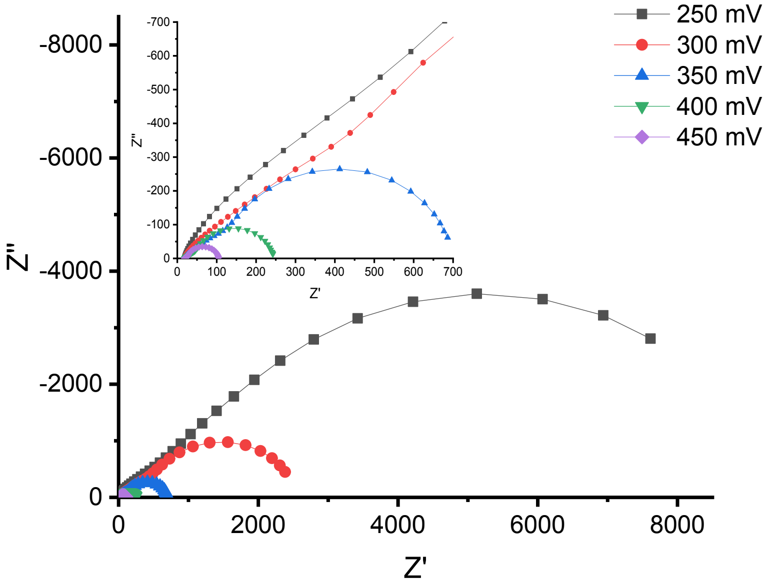


Figure S37 Complex plane (Nyquist) plots of ARM7 sensitized solar cell in the presence of *electrolyte 2*. Plots were recorded in the dark by biasing the cell at forward voltage in the 250-450 mV interval. Inset reports the magnified view of the small arcs obtained at a voltage ≥ 350 mV.

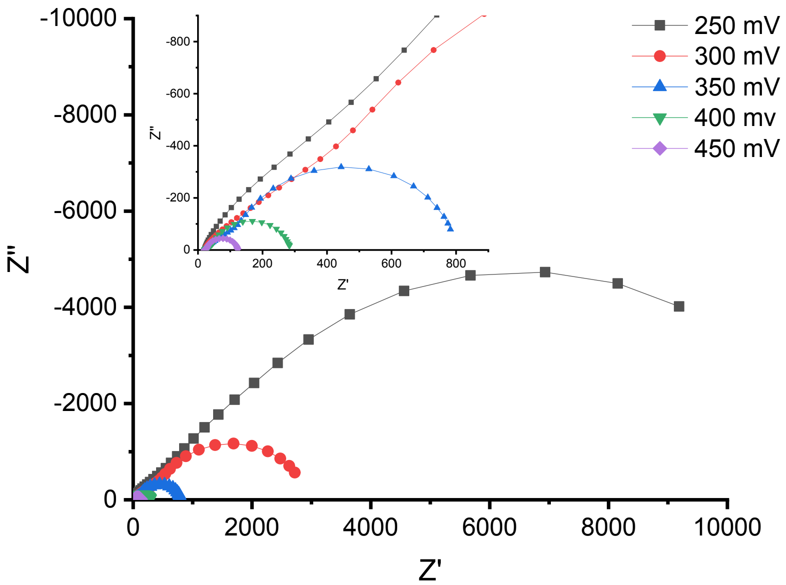


Figure S38 Complex plane (Nyquist) plots of ARM11 sensitized solar cell in the presence of electrolyte 2. Plots were recorded in the dark by biasing the cell at forward voltage in the 250-450 mV interval. Inset reports the magnified view of the small arcs obtained at a voltage ≥ 350 mV.

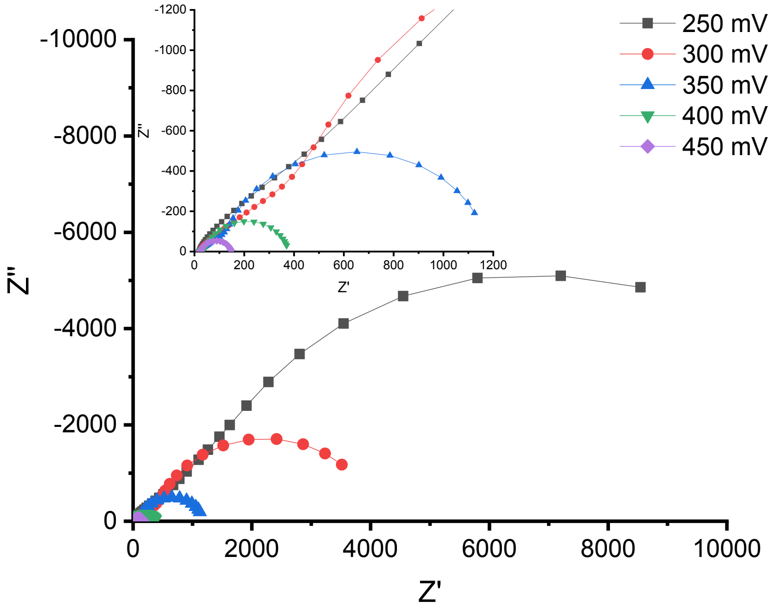


Figure S39 Complex plane (Nyquist) plots of ARM13 sensitized solar cell in the presence of *electrolyte 2*. Plots were recorded in the dark by biasing the cell at forward voltage in the 250-450 mV interval. Inset reports the magnified view of the small arcs obtained at a voltage ≥ 350 mV.

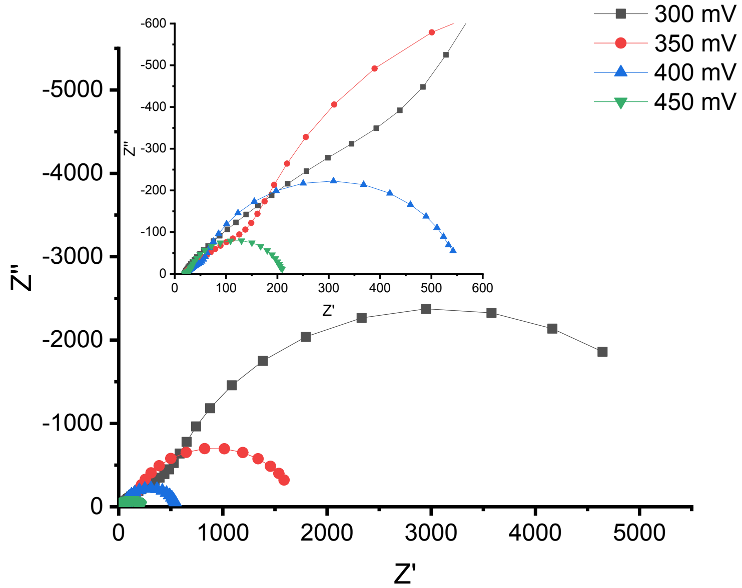


Figure S40 Complex plane (Nyquist) plots of C1 sensitized solar cell in the presence of *electrolyte 2*. Plots were recorded in the dark by biasing the cell at forward voltage in the 300-450 mV interval. Inset reports the magnified view of the small arcs obtained at a voltage ≥ 400 mV.

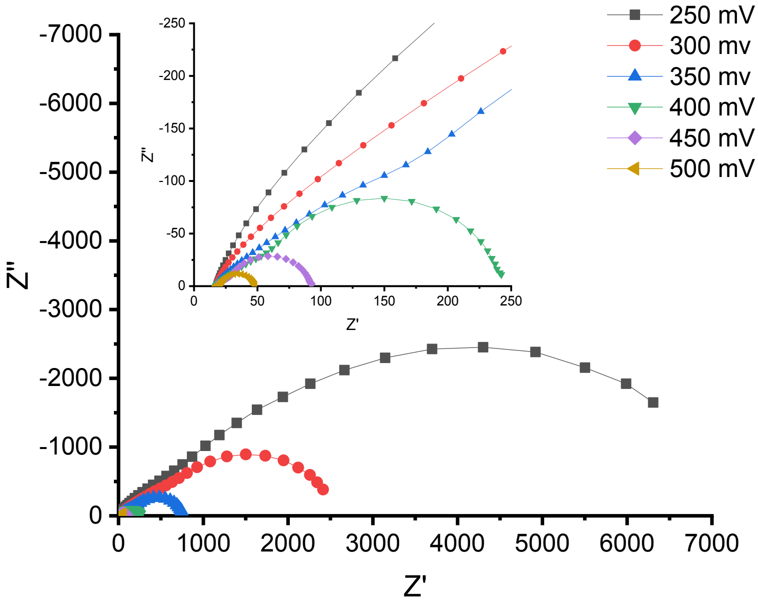


Figure S41 Complex plane (Nyquist) plots of N719 sensitized solar cell in the presence of *electrolyte 2*. Plots were recorded in the dark by biasing the cell at forward voltage in the 250-500 mV interval. Inset reports the magnified view of the small arcs obtained at a voltage ≥ 400 mV.

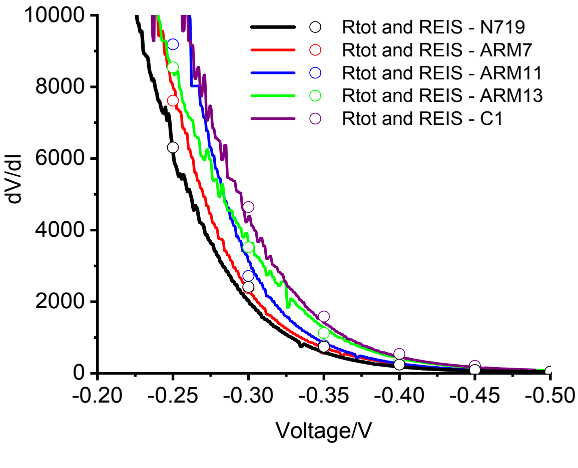


Figure S42 : $R_{TOT} = \frac{\partial V}{\partial J}$ showing a good agreement with RTOT extracted from the fitting of EIS data obtained by sampling the forward voltage at 50 mV intervals under dark conditions

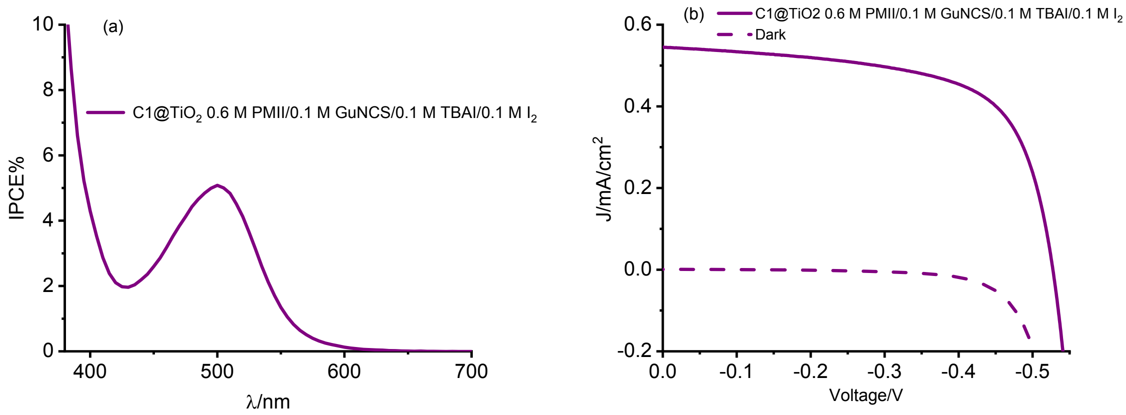


Figure S43 (a) IPCE and (b) JV curves obtained for C1 sensitized cells with *electrolyte 3* deprived of Li^+ and Mg^{2+}.

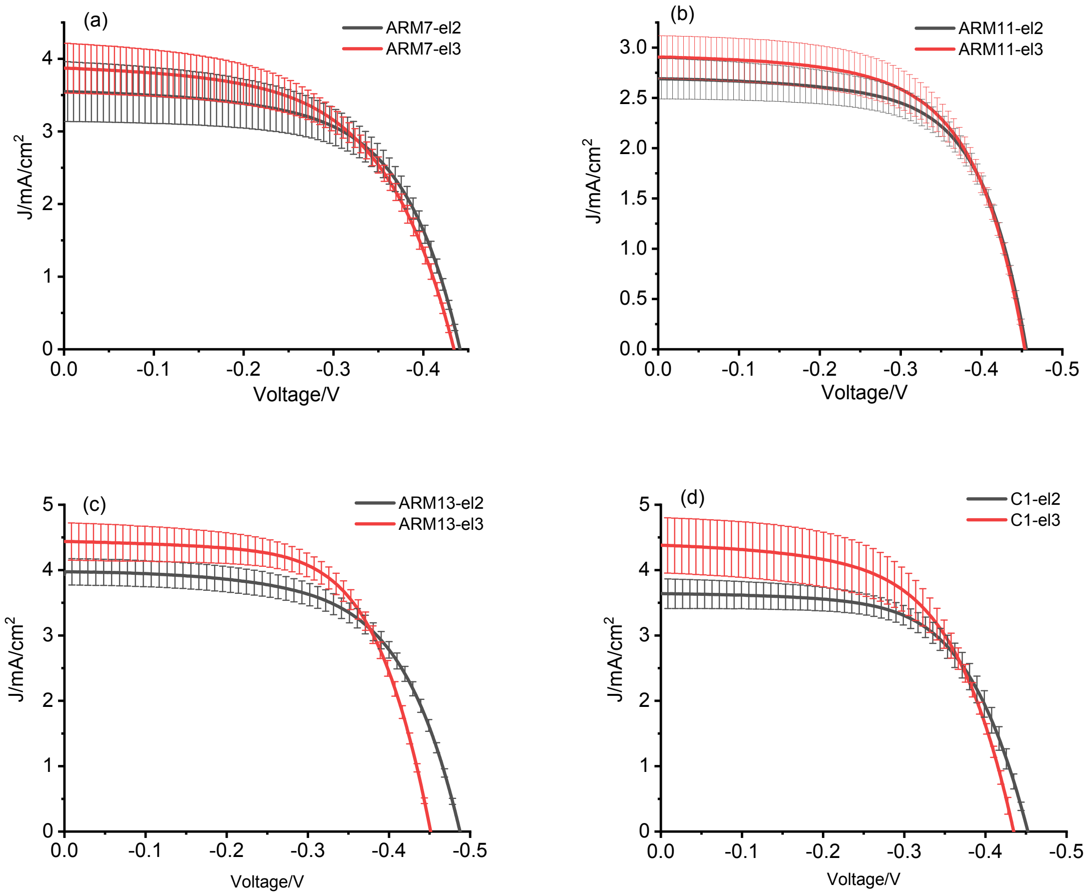


Figure S44 Comparison between JV curves obtained with *el2* and with *el3* for ARM7 (a), ARM11 (b), ARM13 (c) and C1 (d)

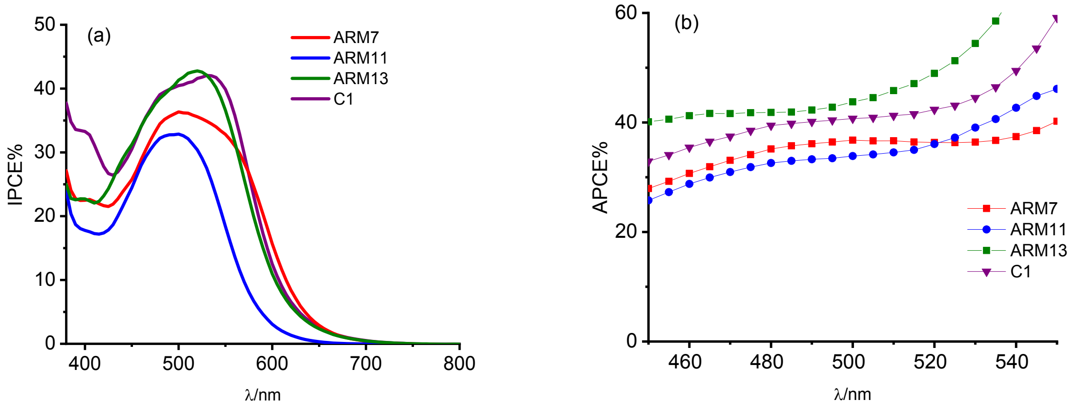


Figure S45: (a), IPCE curves obtained with *electrolyte 3* and Fe(II)NHC sensitized cells. (b), APCE curves obtained from IPCE, The tendency to diverge at low λ is generated by errors in a proper estimation of the optical density of the electrode when the absorbance decreases sharply from the maximum around 500 nm

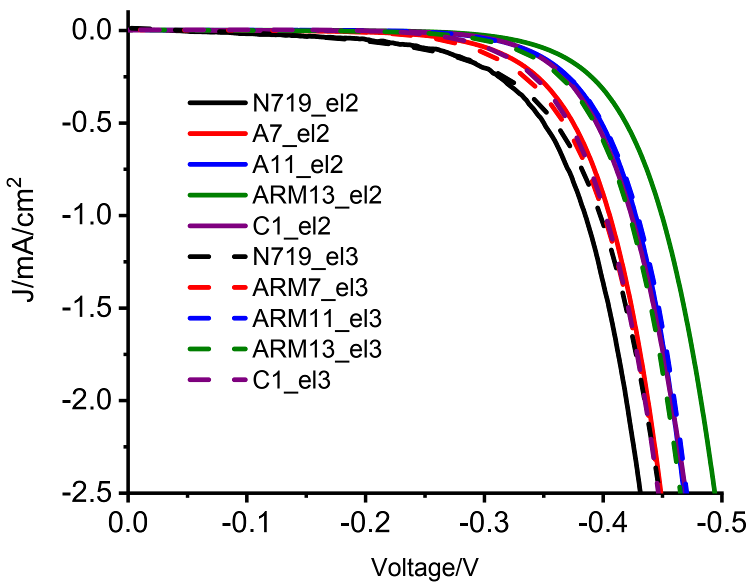


Figure S46: Dark currents of Fe(II)NHC sensitized TiO_2 in contact with *electrolyte 2* (solid line) and *electrolyte3* (dashed lines)

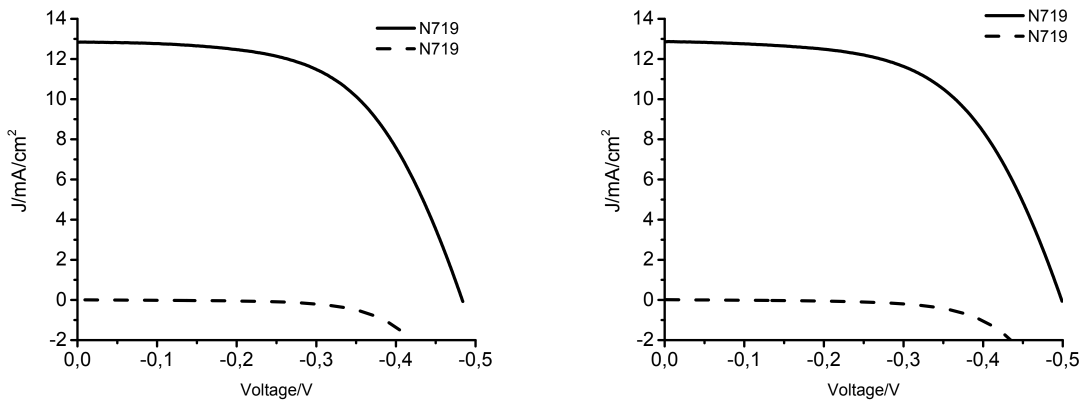


Figure S47: J-V for curves for N719-sensitized DSSCs. Left: with *el2* under AM 1.5 illumination (solid lines) and in the dark (dashed lines). Right : with *electrolyte 3* under AM 1.5 G illumination (solid lines) and in dark conditions (dashed lines).

Cartesian coordinates for ARM13@Mg-TiO_2 and C1@Mg-TiO_2

Table S6: Cartesian coordinates for ARM13@Mg-TiO_2 and C1@Mg-TiO_2 geometries as represented in a xyz file format.

ARM13@Mg-TiO_2

313

H	-7.936	-1.180	8.660
H	-5.810	0.114	8.789
H	-3.638	1.252	8.501
C	-6.071	-0.419	7.877
C	-7.272	-1.132	7.797
C	-3.313	1.038	7.490
H	-3.081	-3.714	7.329
H	-1.383	2.054	7.092
C	-2.216	1.427	6.799
C	-5.248	-0.414	6.765
C	-7.614	-1.819	6.624
N	-4.037	0.240	6.613
H	-4.558	-3.064	6.555
H	-8.542	-2.380	6.544
C	-3.757	-3.802	6.467
H	-4.190	-4.808	6.433
N	-5.558	-1.072	5.623
C	-6.722	-1.760	5.568
N	-2.292	0.860	5.525
C	-3.410	0.119	5.378
H	-1.626	-5.204	5.375
N	-3.015	-3.545	5.238
H	-6.921	0.853	5.110

H	-0.309	0.676	4.870
H	-7.049	2.617	4.864
C	-1.954	-4.341	4.808
C	-1.265	1.076	4.511
C	-3.240	-2.529	4.383
H	-8.713	-3.493	4.379
C	-7.101	1.637	4.374
N	-6.846	-2.371	4.333
H	-1.172	2.150	4.309
Fe	-4.400	-0.993	4.102
H	-8.090	1.492	3.921
C	-7.828	-3.209	3.823
C	-1.485	-3.822	3.645
H	-1.555	0.558	3.596
C	-5.813	-2.160	3.428
N	-2.285	-2.711	3.388
N	-6.079	1.559	3.334
C	-5.124	0.609	3.228
H	-0.670	-4.141	3.009
C	-7.401	-3.548	2.583
N	-3.243	-0.853	2.577
N	-6.179	-2.913	2.367
C	-2.270	-1.773	2.360
C	-5.997	2.485	2.293
H	-6.687	3.318	2.216
N	-4.437	0.976	2.078
H	-7.845	-4.200	1.839
C	-3.369	0.175	1.707
C	-4.959	2.124	1.500
C	-1.426	-1.716	1.258
H	-4.446	-2.583	1.254
C	-5.367	-3.166	1.183
H	-5.130	-4.236	1.174
H	-0.673	-2.477	1.076
C	-2.509	0.370	0.641
H	-4.556	2.572	0.600
C	-1.533	-0.603	0.409
H	-5.921	-2.882	0.279
H	-2.611	1.217	-0.034
C	-0.652	-0.450	-0.800
O	-0.248	-1.571	-1.253
O	-0.478	0.711	-1.287
Mg	-2.421	-2.187	-1.380
H	-3.459	6.467	-1.700
O	-3.317	-4.384	-2.267
O	2.191	-5.742	-2.285
O	-3.303	-0.560	-2.334
O	-3.479	3.003	-2.337
O	-0.166	-7.579	-2.344
O	-3.670	7.121	-2.406
O	7.163	0.117	-2.418
O	2.124	-2.255	-2.427
O	6.041	-5.178	-2.429

O	1.884	1.539	-2.554
O	-3.609	10.679	-2.602
O	1.620	5.111	-2.684
O	4.532	12.057	-2.695
O	-5.325	4.942	-2.727
O	-3.416	-8.238	-2.750
O	7.689	-3.010	-2.751
O	1.490	8.835	-2.763
O	7.009	10.667	-2.820
O	-0.176	-4.150	-2.909
O	5.064	-1.942	-2.917
O	7.034	3.567	-2.940
O	-5.422	-2.488	-2.956
O	6.909	6.970	-2.965
O	7.958	-7.377	-2.970
O	4.557	8.707	-2.976
Ti	0.524	-5.946	-2.987
O	-5.501	1.177	-2.992
O	4.833	1.670	-3.129
O	4.637	5.192	-3.144
Ti	0.385	-2.248	-3.155
Ti	-4.911	-0.617	-3.169
O	-0.471	3.236	-3.181
O	1.416	12.783	-3.241
Ti	-4.855	-4.277	-3.246
Ti	6.073	-3.460	-3.264
Ti	-5.205	3.127	-3.266
Ti	5.249	10.445	-3.269
Ti	6.217	-6.708	-3.277
O	-6.995	-4.446	-3.285
Ti	0.183	1.358	-3.294
O	-0.619	6.923	-3.299
Ti	5.546	-0.098	-3.335
Ti	-1.696	-7.794	-3.344
O	-7.101	-0.705	-3.353
Ti	-5.407	6.615	-3.361
O	-7.311	6.541	-3.386
O	-8.584	9.676	-3.430
Ti	-5.237	10.364	-3.442
O	-6.821	-7.908	-3.452
O	-5.916	8.682	-3.491
O	-6.572	11.668	-3.504
Ti	5.232	6.950	-3.522
Ti	5.382	3.441	-3.524
Ti	-0.006	5.065	-3.545
O	4.448	-7.135	-3.568
O	-7.096	2.974	-3.601
O	-1.667	-2.362	-3.617
Ti	-2.079	-4.170	-3.651
O	-0.159	-0.491	-3.661
Ti	-0.113	8.743	-3.726
Ti	-4.953	-7.953	-3.750
Ti	-2.426	3.111	-3.752

O	-1.634	-6.055	-3.819
Ti	3.098	12.304	-3.836
O	-2.096	5.071	-3.839
Ti	-7.302	-2.479	-3.848
O	-1.836	1.296	-3.850
Ti	-2.217	-0.538	-3.861
O	-5.130	-6.152	-3.867
Ti	3.201	-5.780	-3.880
O	-0.424	10.677	-3.921
Ti	-7.369	1.221	-3.929
Ti	8.214	0.193	-3.927
O	3.883	-4.071	-3.938
Ti	3.134	-2.219	-3.939
O	-1.999	12.600	-3.982
O	-2.091	8.796	-4.005
O	3.553	-0.334	-4.011
Ti	-7.230	-6.185	-4.033
Ti	-2.496	6.895	-4.034
Ti	-2.510	10.788	-4.090
Ti	2.890	1.458	-4.093
Ti	2.667	8.704	-4.154
Ti	-7.993	7.992	-4.159
Ti	2.731	5.082	-4.169
O	9.256	-1.308	-4.169
Ti	-8.228	11.226	-4.174
O	9.362	-4.818	-4.210
Ti	-0.156	12.476	-4.213
O	3.232	6.946	-4.217
O	8.862	1.906	-4.261
O	3.330	3.347	-4.282
O	3.249	10.544	-4.328
O	8.627	8.647	-4.329
Ti	8.854	-6.573	-4.358
O	8.715	5.298	-4.407
Ti	7.867	10.252	-4.441
O	-8.993	-2.525	-4.450
Ti	8.662	-3.065	-4.489
O	-9.098	1.101	-4.536
O	1.351	-6.151	-4.610
Ti	7.935	6.915	-4.657
Ti	8.081	3.532	-4.669
O	-3.863	-4.011	-4.696
O	-4.007	-0.644	-4.742
O	-9.631	7.491	-4.773
O	1.405	-2.417	-4.772
O	-4.200	3.145	-4.779
O	-8.912	-6.423	-4.803
O	6.594	-0.074	-4.817
O	-4.350	6.713	-4.874
O	1.181	1.421	-4.912
O	6.984	-6.158	-4.976
O	-1.244	-8.492	-4.995
O	-4.276	10.600	-4.999

O	-9.787	11.902	-5.023
O	6.014	10.118	-5.036
O	6.723	-3.392	-5.042
O	0.923	5.111	-5.087
O	0.882	8.574	-5.183
O	6.125	3.454	-5.266
O	5.989	6.939	-5.300
O	3.678	13.070	-5.412
O	-4.565	-8.556	-5.442
O	-6.801	-2.409	-5.704
O	-1.699	-4.097	-5.707
O	-6.914	1.063	-5.780
O	0.322	13.036	-5.879
O	3.439	-6.139	-5.885
O	-6.850	-5.567	-5.902
O	-1.777	-0.630	-5.905
O	-1.920	3.126	-5.910
O	8.954	-7.425	-5.974
O	-7.788	10.679	-6.000
O	-7.510	7.944	-6.024
O	-2.100	6.883	-6.032
O	3.599	-2.172	-6.071
O	8.073	10.989	-6.132
O	3.444	1.340	-6.199
O	-7.400	4.597	-6.235
O	3.043	8.566	-6.247
O	-2.183	10.631	-6.266
O	3.187	5.167	-6.308
Ti	-8.742	-2.369	-6.362
O	8.815	-2.994	-6.360
Ti	-8.865	1.019	-6.410
Ti	-8.691	-5.705	-6.501
O	8.290	3.493	-6.545
O	8.165	7.115	-6.573
O	-4.082	-6.051	-6.582
Ti	-9.442	7.600	-6.646
O	-9.498	-0.736	-6.659
Ti	-9.643	11.105	-6.660
O	-9.445	-4.095	-6.662
Ti	-0.707	-7.990	-6.665
Ti	-3.456	-4.231	-6.769
O	-4.084	1.165	-6.769
Ti	1.668	-6.351	-6.771
Ti	7.384	-6.755	-6.798
O	-4.021	-2.458	-6.811
O	1.273	-4.348	-6.828
O	1.133	-8.163	-6.839
O	-9.650	2.637	-6.860
Ti	-3.704	3.020	-6.866
Ti	6.385	10.765	-6.885
Ti	-3.505	-0.619	-6.897
O	-10.129	9.344	-6.901
O	-4.330	4.854	-6.903

Ti	7.153	-3.522	-6.935
Ti	1.794	-2.465	-6.939
O	-10.036	5.847	-6.983
Ti	-3.978	6.711	-6.988
O	-0.406	-6.210	-6.989
O	-4.669	8.562	-6.991
O	0.791	10.580	-7.004
Ti	-4.010	10.302	-7.013
Ti	-3.952	-7.827	-7.031
O	1.269	-0.563	-7.039
O	1.033	3.213	-7.060
O	4.282	10.720	-7.091
Ti	1.657	1.348	-7.103
Ti	4.090	12.515	-7.118
Ti	6.551	3.319	-7.126
Ti	-0.661	-4.238	-7.147
Ti	6.474	7.049	-7.157
Ti	-8.996	4.344	-7.183
Ti	1.424	5.039	-7.229
Ti	1.275	8.722	-7.259
O	0.856	6.888	-7.281
O	-5.227	11.687	-7.298
Ti	-0.725	-0.599	-7.377
O	5.961	12.511	-7.386
O	5.713	-7.235	-7.411
Ti	-0.962	3.086	-7.423
O	5.076	-4.257	-7.435
Ti	4.383	-5.926	-7.459
Ti	-6.031	-2.457	-7.473
O	6.309	1.579	-7.482
Ti	-6.147	1.061	-7.509
Ti	0.845	12.323	-7.506
Ti	-1.165	6.795	-7.595
O	7.740	-5.244	-7.608
O	-0.176	-2.456	-7.609
O	-2.282	-8.322	-7.637
Ti	-6.073	-5.952	-7.655
Ti	4.501	-2.193	-7.657
Ti	-6.980	11.272	-7.663
O	6.265	5.277	-7.669
O	6.142	9.037	-7.671
Ti	-6.308	4.614	-7.680
O	-0.342	1.258	-7.694
Ti	4.034	8.824	-7.711
Ti	4.402	1.326	-7.754
Ti	-6.803	8.012	-7.771
O	-0.583	4.980	-7.813
O	6.473	-2.162	-7.818
O	-5.561	2.863	-7.862
Ti	4.137	5.138	-7.867
O	-5.433	-0.692	-7.873
Ti	-1.342	10.453	-7.898
O	-5.382	-4.231	-7.982

O	-8.711	11.952	-7.992
O	-0.634	8.673	-8.019
O	4.683	3.366	-8.033
O	-7.703	-2.454	-8.045
O	-5.762	6.470	-8.050
O	4.585	7.063	-8.050
O	-7.837	-6.180	-8.102
O	2.537	12.811	-8.104
O	-7.786	0.999	-8.126
O	-2.273	-4.374	-8.134
O	-5.363	-7.583	-8.193
O	4.525	-0.443	-8.240
O	2.740	-6.266	-8.273
O	-2.359	-0.640	-8.318
O	-2.588	3.021	-8.324
O	-8.396	7.544	-8.337
O	2.830	-2.647	-8.418
O	-2.822	6.773	-8.427
O	-6.767	9.752	-8.531
O	-0.649	12.072	-8.550
O	2.631	1.510	-8.576
O	-3.013	10.283	-8.601
O	-7.874	4.424	-8.654
O	2.458	8.954	-8.658
O	2.492	5.083	-8.719

C1@Mg-TiO_2
316

O	-7.875	-0.565	10.041
H	-9.813	-1.787	9.643
C	-8.157	-1.134	8.998
O	-9.290	-1.836	8.800
H	-5.810	0.114	8.789
H	-3.638	1.252	8.501
C	-6.071	-0.419	7.877
C	-7.272	-1.132	7.797
C	-3.313	1.038	7.490
H	-3.081	-3.714	7.329
H	-1.383	2.054	7.092
C	-2.216	1.427	6.799
C	-5.248	-0.414	6.765
C	-7.614	-1.819	6.624
N	-4.037	0.240	6.613
H	-4.558	-3.064	6.555
H	-8.542	-2.380	6.544
C	-3.757	-3.802	6.467
H	-4.190	-4.808	6.433
N	-5.558	-1.072	5.623
C	-6.722	-1.760	5.568
N	-2.292	0.860	5.525
C	-3.410	0.119	5.378
H	-1.626	-5.204	5.375

N	-3.015	-3.545	5.238
H	-6.921	0.853	5.110
H	-0.309	0.676	4.870
H	-7.049	2.617	4.864
C	-1.954	-4.341	4.808
C	-1.265	1.076	4.511
C	-3.240	-2.529	4.383
H	-8.713	-3.493	4.379
C	-7.101	1.637	4.374
N	-6.846	-2.371	4.333
H	-1.172	2.150	4.309
Fe	-4.400	-0.993	4.102
H	-8.090	1.492	3.921
C	-7.828	-3.209	3.823
C	-1.485	-3.822	3.645
H	-1.555	0.558	3.596
C	-5.813	-2.160	3.428
N	-2.285	-2.711	3.388
N	-6.079	1.559	3.334
C	-5.124	0.609	3.228
H	-0.670	-4.141	3.009
C	-7.401	-3.548	2.583
N	-3.243	-0.853	2.577
N	-6.179	-2.913	2.367
C	-2.270	-1.773	2.360
C	-5.997	2.485	2.293
H	-6.687	3.318	2.216
N	-4.437	0.976	2.078
H	-7.845	-4.200	1.839
C	-3.369	0.175	1.707
C	-4.959	2.124	1.500
C	-1.426	-1.716	1.258
H	-4.446	-2.583	1.254
C	-5.367	-3.166	1.183
H	-5.130	-4.236	1.174
H	-0.673	-2.477	1.076
C	-2.509	0.370	0.641
H	-4.556	2.572	0.600
C	-1.533	-0.603	0.409
H	-5.921	-2.882	0.279
H	-2.611	1.217	-0.034
C	-0.652	-0.450	-0.800
O	-0.248	-1.571	-1.253
O	-0.478	0.711	-1.287
MG	-2.421	-2.187	-1.380
H	-3.459	6.467	-1.700
O	-3.317	-4.384	-2.267
O	2.191	-5.742	-2.285
O	-3.303	-0.560	-2.334
O	-3.479	3.003	-2.337
O	-0.166	-7.579	-2.344
O	-3.670	7.121	-2.406
O	7.163	0.117	-2.418

O	2.124	-2.255	-2.427
O	6.041	-5.178	-2.429
O	1.884	1.539	-2.554
O	-3.609	10.679	-2.602
O	1.620	5.111	-2.684
O	4.532	12.057	-2.695
O	-5.325	4.942	-2.727
O	-3.416	-8.238	-2.750
O	7.689	-3.010	-2.751
O	1.490	8.835	-2.763
O	7.009	10.667	-2.820
O	-0.176	-4.150	-2.909
O	5.064	-1.942	-2.917
O	7.034	3.567	-2.940
O	-5.422	-2.488	-2.956
O	6.909	6.970	-2.965
O	7.958	-7.377	-2.970
O	4.557	8.707	-2.976
Ti	0.524	-5.946	-2.987
O	-5.501	1.177	-2.992
O	4.833	1.670	-3.129
O	4.637	5.192	-3.144
Ti	0.385	-2.248	-3.155
Ti	-4.911	-0.617	-3.169
O	-0.471	3.236	-3.181
O	1.416	12.783	-3.241
Ti	-4.855	-4.277	-3.246
Ti	6.073	-3.460	-3.264
Ti	-5.205	3.127	-3.266
Ti	5.249	10.445	-3.269
Ti	6.217	-6.708	-3.277
O	-6.995	-4.446	-3.285
Ti	0.183	1.358	-3.294
O	-0.619	6.923	-3.299
Ti	5.546	-0.098	-3.335
Ti	-1.696	-7.794	-3.344
O	-7.101	-0.705	-3.353
Ti	-5.407	6.615	-3.361
O	-7.311	6.541	-3.386
O	-8.584	9.676	-3.430
Ti	-5.237	10.364	-3.442
O	-6.821	-7.908	-3.452
O	-5.916	8.682	-3.491
O	-6.572	11.668	-3.504
Ti	5.232	6.950	-3.522
Ti	5.382	3.441	-3.524
Ti	-0.006	5.065	-3.545
O	4.448	-7.135	-3.568
O	-7.096	2.974	-3.601
O	-1.667	-2.362	-3.617
Ti	-2.079	-4.170	-3.651
O	-0.159	-0.491	-3.661
Ti	-0.113	8.743	-3.726

Ti	-4.953	-7.953	-3.750
Ti	-2.426	3.111	-3.752
O	-1.634	-6.055	-3.819
Ti	3.098	12.304	-3.836
O	-2.096	5.071	-3.839
Ti	-7.302	-2.479	-3.848
O	-1.836	1.296	-3.850
Ti	-2.217	-0.538	-3.861
O	-5.130	-6.152	-3.867
Ti	3.201	-5.780	-3.880
O	-0.424	10.677	-3.921
Ti	-7.369	1.221	-3.929
Ti	8.214	0.193	-3.927
O	3.883	-4.071	-3.938
Ti	3.134	-2.219	-3.939
O	-1.999	12.600	-3.982
O	-2.091	8.796	-4.005
O	3.553	-0.334	-4.011
Ti	-7.230	-6.185	-4.033
Ti	-2.496	6.895	-4.034
Ti	-2.510	10.788	-4.090
Ti	2.890	1.458	-4.093
Ti	2.667	8.704	-4.154
Ti	-7.993	7.992	-4.159
Ti	2.731	5.082	-4.169
O	9.256	-1.308	-4.169
Ti	-8.228	11.226	-4.174
O	9.362	-4.818	-4.210
Ti	-0.156	12.476	-4.213
O	3.232	6.946	-4.217
O	8.862	1.906	-4.261
O	3.330	3.347	-4.282
O	3.249	10.544	-4.328
O	8.627	8.647	-4.329
Ti	8.854	-6.573	-4.358
O	8.715	5.298	-4.407
Ti	7.867	10.252	-4.441
O	-8.993	-2.525	-4.450
Ti	8.662	-3.065	-4.489
O	-9.098	1.101	-4.536
O	1.351	-6.151	-4.610
Ti	7.935	6.915	-4.657
Ti	8.081	3.532	-4.669
O	-3.863	-4.011	-4.696
O	-4.007	-0.644	-4.742
O	-9.631	7.491	-4.773
O	1.405	-2.417	-4.772
O	-4.200	3.145	-4.779
O	-8.912	-6.423	-4.803
O	6.594	-0.074	-4.817
O	-4.350	6.713	-4.874
O	1.181	1.421	-4.912
O	6.984	-6.158	-4.976

O	-1.244	-8.492	-4.995
O	-4.276	10.600	-4.999
O	-9.787	11.902	-5.023
O	6.014	10.118	-5.036
O	6.723	-3.392	-5.042
O	0.923	5.111	-5.087
O	0.882	8.574	-5.183
O	6.125	3.454	-5.266
O	5.989	6.939	-5.300
O	3.678	13.070	-5.412
O	-4.565	-8.556	-5.442
O	-6.801	-2.409	-5.704
O	-1.699	-4.097	-5.707
O	-6.914	1.063	-5.780
O	0.322	13.036	-5.879
O	3.439	-6.139	-5.885
O	-6.850	-5.567	-5.902
O	-1.777	-0.630	-5.905
O	-1.920	3.126	-5.910
O	8.954	-7.425	-5.974
O	-7.788	10.679	-6.000
O	-7.510	7.944	-6.024
O	-2.100	6.883	-6.032
O	3.599	-2.172	-6.071
O	8.073	10.989	-6.132
O	3.444	1.340	-6.199
O	-7.400	4.597	-6.235
O	3.043	8.566	-6.247
O	-2.183	10.631	-6.266
O	3.187	5.167	-6.308
Ti	-8.742	-2.369	-6.362
O	8.815	-2.994	-6.360
Ti	-8.865	1.019	-6.410
Ti	-8.691	-5.705	-6.501
O	8.290	3.493	-6.545
O	8.165	7.115	-6.573
O	-4.082	-6.051	-6.582
Ti	-9.442	7.600	-6.646
O	-9.498	-0.736	-6.659
Ti	-9.643	11.105	-6.660
O	-9.445	-4.095	-6.662
Ti	-0.707	-7.990	-6.665
Ti	-3.456	-4.231	-6.769
O	-4.084	1.165	-6.769
Ti	1.668	-6.351	-6.771
Ti	7.384	-6.755	-6.798
O	-4.021	-2.458	-6.811
O	1.273	-4.348	-6.828
O	1.133	-8.163	-6.839
O	-9.650	2.637	-6.860
Ti	-3.704	3.020	-6.866
Ti	6.385	10.765	-6.885
Ti	-3.505	-0.619	-6.897

O	-10.129	9.344	-6.901
O	-4.330	4.854	-6.903
Ti	7.153	-3.522	-6.935
Ti	1.794	-2.465	-6.939
O	-10.036	5.847	-6.983
Ti	-3.978	6.711	-6.988
O	-0.406	-6.210	-6.989
O	-4.669	8.562	-6.991
O	0.791	10.580	-7.004
Ti	-4.010	10.302	-7.013
Ti	-3.952	-7.827	-7.031
O	1.269	-0.563	-7.039
O	1.033	3.213	-7.060
O	4.282	10.720	-7.091
Ti	1.657	1.348	-7.103
Ti	4.090	12.515	-7.118
Ti	6.551	3.319	-7.126
Ti	-0.661	-4.238	-7.147
Ti	6.474	7.049	-7.157
Ti	-8.996	4.344	-7.183
Ti	1.424	5.039	-7.229
Ti	1.275	8.722	-7.259
O	0.856	6.888	-7.281
O	-5.227	11.687	-7.298
Ti	-0.725	-0.599	-7.377
O	5.961	12.511	-7.386
O	5.713	-7.235	-7.411
Ti	-0.962	3.086	-7.423
O	5.076	-4.257	-7.435
Ti	4.383	-5.926	-7.459
Ti	-6.031	-2.457	-7.473
O	6.309	1.579	-7.482
Ti	-6.147	1.061	-7.509
Ti	0.845	12.323	-7.506
Ti	-1.165	6.795	-7.595
O	7.740	-5.244	-7.608
O	-0.176	-2.456	-7.609
O	-2.282	-8.322	-7.637
Ti	-6.073	-5.952	-7.655
Ti	4.501	-2.193	-7.657
Ti	-6.980	11.272	-7.663
O	6.265	5.277	-7.669
O	6.142	9.037	-7.671
Ti	-6.308	4.614	-7.680
O	-0.342	1.258	-7.694
Ti	4.034	8.824	-7.711
Ti	4.402	1.326	-7.754
Ti	-6.803	8.012	-7.771
O	-0.583	4.980	-7.813
O	6.473	-2.162	-7.818
O	-5.561	2.863	-7.862
Ti	4.137	5.138	-7.867
O	-5.433	-0.692	-7.873

Ti	-1.342	10.453	-7.898
O	-5.382	-4.231	-7.982
O	-8.711	11.952	-7.992
O	-0.634	8.673	-8.019
O	4.683	3.366	-8.033
O	-7.703	-2.454	-8.045
O	-5.762	6.470	-8.050
O	4.585	7.063	-8.050
O	-7.837	-6.180	-8.102
O	2.537	12.811	-8.104
O	-7.786	0.999	-8.126
O	-2.273	-4.374	-8.134
O	-5.363	-7.583	-8.193
O	4.525	-0.443	-8.240
O	2.740	-6.266	-8.273
O	-2.359	-0.640	-8.318
O	-2.588	3.021	-8.324
O	-8.396	7.544	-8.337
O	2.830	-2.647	-8.418
O	-2.822	6.773	-8.427
O	-6.767	9.752	-8.531
O	-0.649	12.072	-8.550
O	2.631	1.510	-8.576
O	-3.013	10.283	-8.601
O	-7.874	4.424	-8.654
O	2.458	8.954	-8.658
O	2.492	5.083	-8.719