Electronic Supplementary Material (ESI) for RSC Advances.

Stability of ruthenium/organic dye co-sensitized solar cells: A joint experimental and computational investigation

Paolo Salvatori, Saurabh Agrawal, Chiranjeevi Barreddi, Chandrasekharam Malapaka, Mervyn de Borniol, Filippo De Angelis,**

Electronic Supplementary Materials

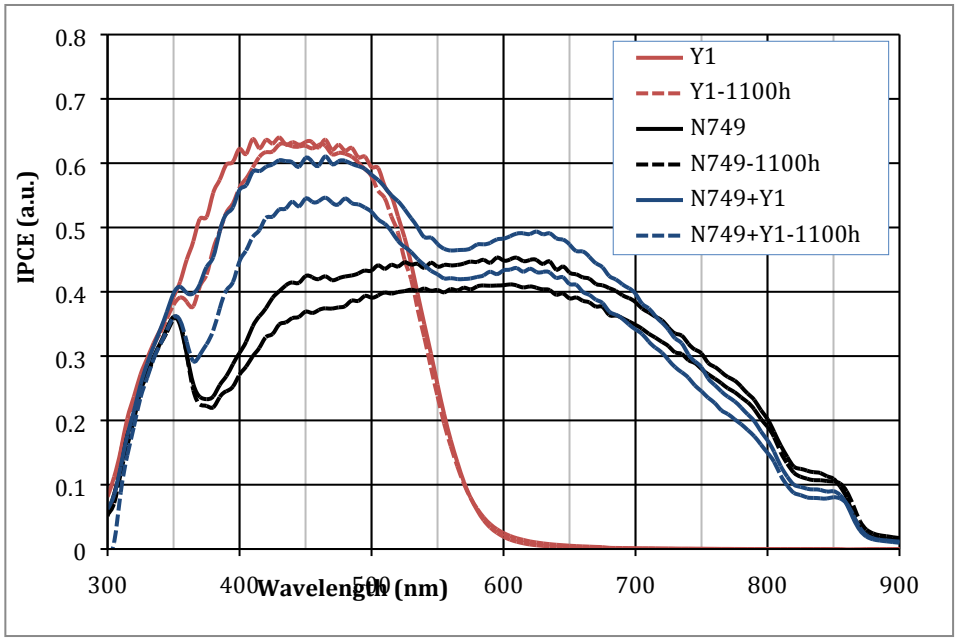

Figure S1. IPCE spectra forY1, N749 and N749-Y1 cocktail dyes before and after ageing test.

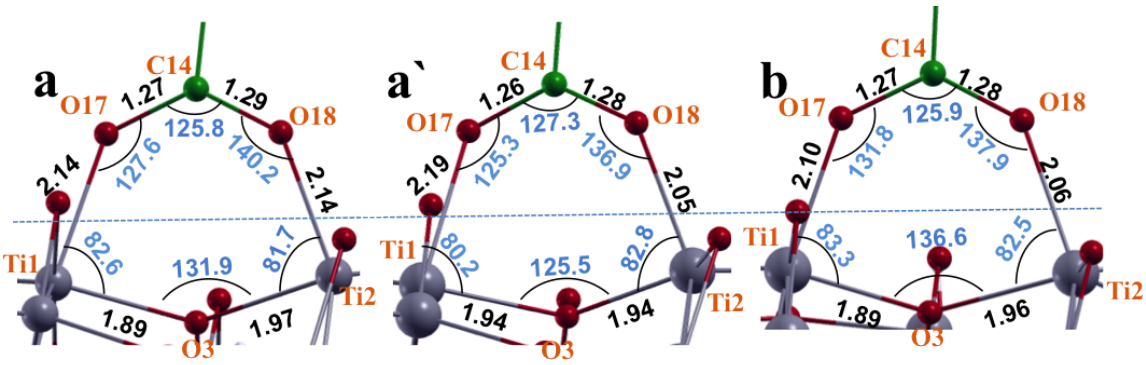

Figure S2. Structural details of the dye@TiO_2 interface. (a) Y1@TiO_2, (a`) $Y1^{ox}$@TiO_2 and (b) Y2@TiO_2.

Table S1. Main geometrical parameters for organic dye@TiO_2 interfaces.

Bond Distances (Å) and angles	**Y1@TiO_2**	**Y1^{ox}@TiO_2**	**Y2@TiO_2**
C14-O17	1.27	1.26	1.27
C14-O18	1.29	1.28	1.28
O17-Ti1	2.14	2.19	2.10
O18-Ti2	2.01	2.05	2.06
Ti1-O3	1.89	1.94	1.89
Ti2-O3	1.97	1.94	1.96
O17-Ti1-O3	82.6˚	80.2 ˚	83.3 ˚
Ti1-O3-Ti2	131.9 ˚	125.5 ˚	136.6 ˚
O18-Ti2-O3	81.7 ˚	82.8 ˚	82.5 ˚
O17-C14-O18	125.8 ˚	127.3 ˚	125.9 ˚
Ti1-O17-C14	127.6 ˚	125.3 ˚	131.8 ˚
Ti2-O18-C14	140.2 ˚	136.9 ˚	137.9 ˚

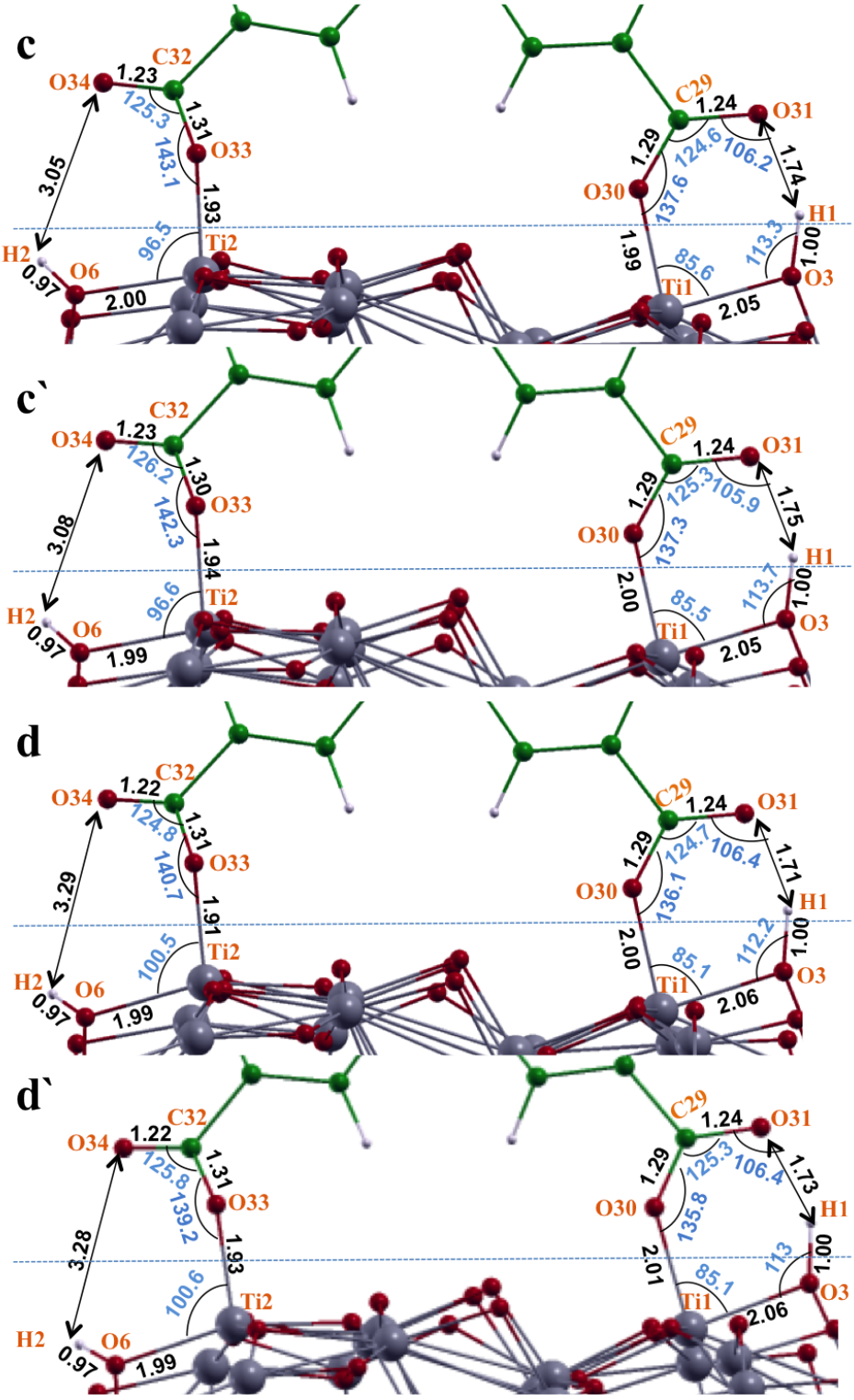

Figure S3. Structural details of the dye@TiO_2 interface. (c) N749@TiO_2, (c`) $[N749]^{ox}$@$TiO_2$, (d) [N749-TBA]@$TiO_2$ and (d`) $[N749\text{-}TBA]^{ox}$@TiO_2.

Table S2. Geometrical parameters for N749@TiO_2 and [N749-TBA]@TiO_2 interfaces.

Bond Distances (Å) and angles	**N749@TiO_2**	**[N749]^{ox}@TiO_2**	**[N749-TBA] @TiO_2**	**[N749-TBA]^{ox} @TiO_2**
C29-O30	1.29	1.29	1.29	1.29
C29-O31	1.24	1.24	1.24	1.24
O30-Ti1	1.99	2.00	2.00	2.01
O31-H1	1.74	1.75	1.71	1.73
Ti1-O3	2.05	2.05	2.06	2.06
O3-H1	1.00	1.00	1.00	1.00
C32-O33	1.31	1.30	1.31	1.31
C32-O34	1.23	1.23	1.22	1.22
O33-Ti2	1.93	1.94	1.91	1.93
O34-H2	3.05	3.08	3.29	3.28
Ti2-O6	2.00	1.99	1.99	1.99
O6-H2	0.97	0.97	0.97	0.97
O30-C29-O31	124.6 °	125.3 °	124.7 °	125.3 °
Ti1-O30-C29	137.6 °	137.3 °	136.1 °	135.8 °
C29-O31-H1	106.2 °	105.9 °	106.4 °	106.4 °
O30-Ti1-O3	85.6 °	85.5 °	85.1 °	85.1 °
Ti1-O3-H1	113.3 °	113.7 °	112.2 °	113.0 °
O33-C32-O34	125.3 °	126.2 °	124.8 °	125.8 °
Ti2-O33-C32	143.1 °	142.3 °	140.7 °	139.2 °
O33-Ti2-O6	96.5 °	96.6 °	100.5 °	100.6 °

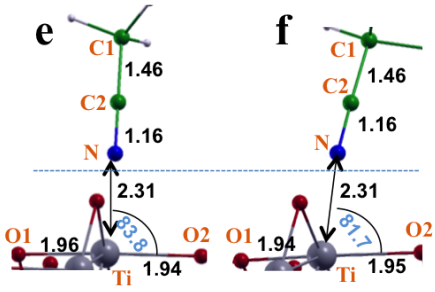

Figure S4. Structural details of the solvent-TiO_2 interface. (e) ACN@TiO_2, (f) MPN@TiO_2.

Table S3. Main geometrical parameters for ACN@TiO_2 and MPN@TiO_2 complexes.

Bond Distances (Å) and angles	**ACN@TiO_2**	**MPN@TiO_2**
C1-C2	1.46	1.46
C2-N	1.16	1.16
N-Ti	2.31	2.31
O1-Ti	1.96	1.94
O2-Ti	1.94	1.95
Ti-N-C2	170.2 °	170.4 °

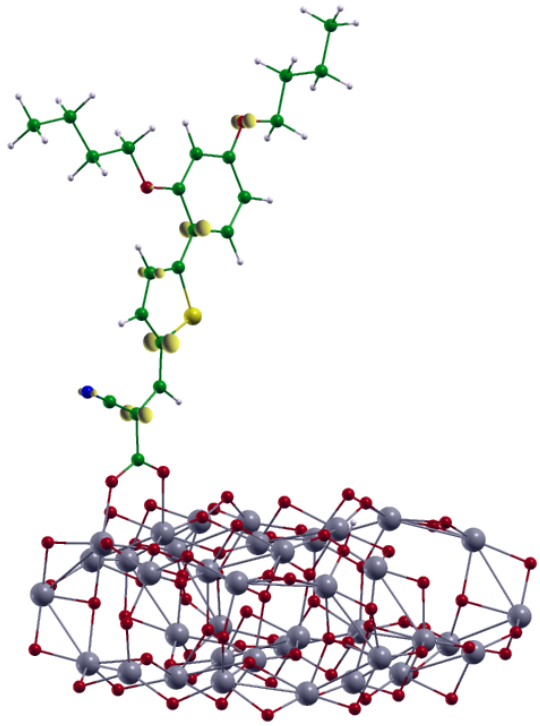

Figure S5. Spin density plots (isovalue 0.02 e/a.u.^{3}) of Y1^{ox}@TiO_2.

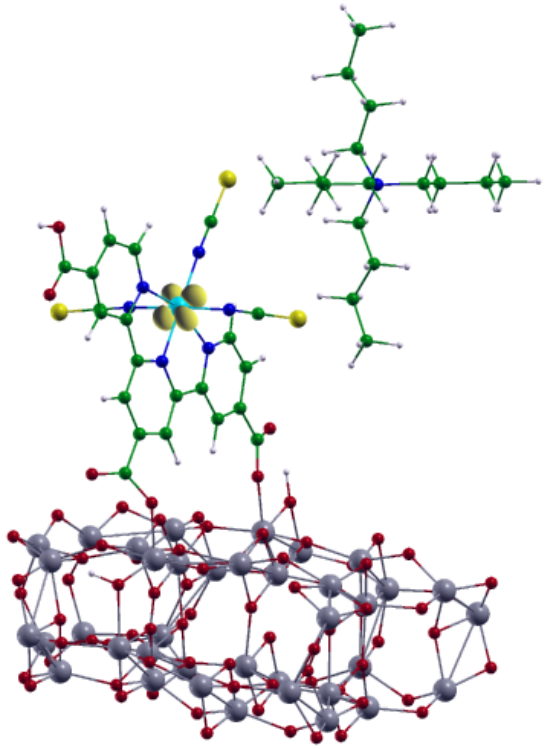

Figure S6. Spin density plots (isovalue 0.02 e/a.u.^{3}) of [N749-TBA]^{ox}@TiO_2.