A study of the impact of co-adsorbents on DSSC electron transfer processes:

anti- -staking vs. shield effect

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Supporting information

Absorption at 539 nm of cells with various co-adsorbent/N719 ratios, and estimated values for surface dye concentration and coverage fractions S2

Current density vs. voltage curves of DSSC prepared with various co-adsorbent/N719 ratios. S3

Absorption at 530 nm of cells with various co-adsorbent/N719 ratios, and estimated values for surface dye concentration (mole cm^{-2}) and coverage fraction of the dye

Variables	Medium	CDCA/N719				
	Pure N719	0.01	0.1	1	10	100
OD at 530 nm	0.901	0.782	0.724	0.684	0.622	0.550
Surf. Concentration	6.34E-08	5.50E-08	5.10E-08	4.82E-08	4.38E-08	3.87E-08
Coverage fraction	48%	41%	36%	36%	33%	29%
		BMPP/N719				
OD at 530 nm		1.037	0.966	0.900	0.810	0.566
Surf. Concentration		7.30E-08	6.8E-08	6.34E-08	5.70E-08	3.99E-08
Coverage fraction		55%	51%	48%	43%	30%

The amount of N719 grafted on the co-adsorbent free cells has been measured after desorption of the dye from the TiO2 layer using 4 M KOH solution, and subsequent measurement of the optical density of the obtained solution at 530 nm, taking into account the value of the molecular extinction coefficient, near 14200. The surface concentration has been calculated dividing this mole amount by the external area of the cell, here 6 x 6 mm².

Because the two co-adsorbents employed are perfectly transparent at the working wavelength, it has been considered that the optical density was solely due to the presence of the dye, whose surface concentration was directly estimated from the DO. Moreover, the projected area of the sensitizer can be estimated from a drawing software to range between 80 and 100 Angström². The surface covered by the dye was calculated from the above surface concentration and the projected area of this molecule, taking into account the Avogadro number.

The real surface of the TiO_2 layer was estimated from the thickness of the layer (5 µm), the surface area of the material, in the order of 50 m²/g and the density of the SC layer, taken at 2.8 g/cm2 from the density of titanium oxide and the porosity of the particle layer. The surface area of TiO_2 substrate was then in the order of 700 cm² cm⁻². The coverage fraction was finally obtained by dividing the two above surface. The values reported in the above tables have to be taken with care, because of the assumptions made; however they can be sued for comparison purpose between the various co-adsorbent ó dye combinations.

Current density vs. voltage curves of DSSC prepared with various co-adsorbent/N719 ratios.

NB. These curves are the average of the data produced with the three replicate cells, for all co-adsorbent-dye combinations.



j vs. V curves with various BMPP amounts

