Adsorption Properties of *p*-Methyl Red Monomeric-to-Pentameric Dye Aggregates on Anatase (101) Titania Surfaces: First Principles Calculations of Dye/TiO_2 Photoanode Interfaces for Dye-Sensitized Solar Cells

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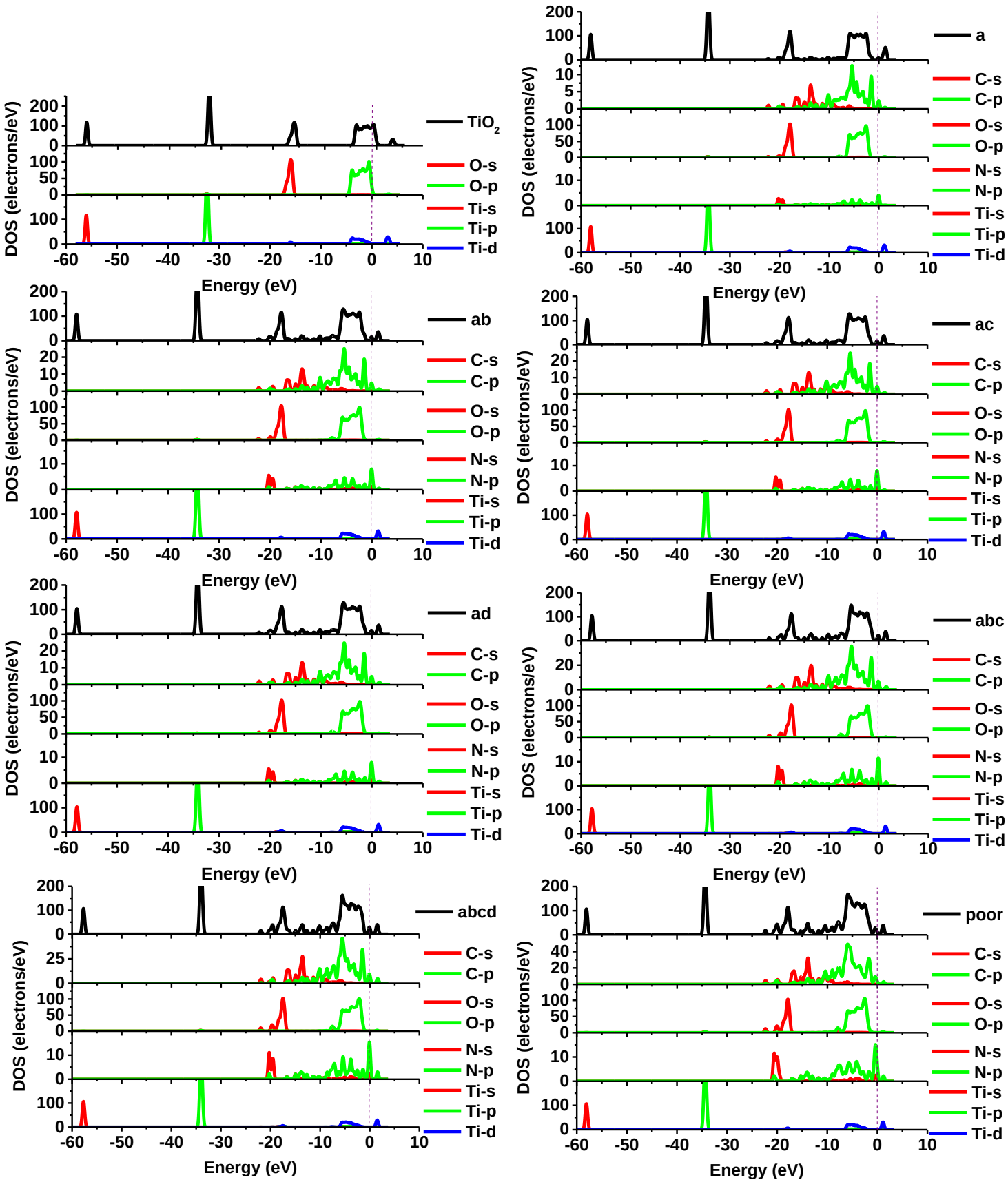
DOS (electrons/eV)
Energy (eV)
TiO2
O-s
O-p
Ti-s
Ti-p
Ti-d
a
C-s
C-p
N-s
N-p
ab
ac
ad
abc
abcd
poor

Figure S1 DOS (black) and PDOS plots of bare "TiO_2" and "a", "ab", "ac", "ad", "abc", "abcd" and "poor" dye adsorbates on the (101) TiO_2 surface, according to their s- (red), p- (green) and, in the case of Ti, d- (blue) orbital contributions.

Table S1 The band gap energies of *p*-methyl red *in vacuo*, "a", "ab", "ac", "ad", "abc", "abcd" and "poor". The energies decrease from 2.82 eV for bare TiO_2 slab to 0.78 eV-1.17 eV for dye/TiO_2 structures

Structure	*p*-methyl red	TiO_2	a	ab	ac	ad	abc	abcd	poor
Band gap (eV)	1.77	2.82	0.78	0.92	0.93	0.97	1.05	1.17	0.79

Table S2 The peak wavelength and intensity of bare "TiO_2", "a", "ab", "ac", "ad", "abc", "abcd" and "poor".

Structure	TiO_2	a	ab	ac	ad	abc	abcd	poor
Peak (nm) [a]	320	319	322	322	322	325	331	328
Intensity (cm^{-1}) [a]	20101	20205	20236	20152	20104	20404	21046	20531
Peak (nm) [b]	-	845	751	751	724	676	633	614
Intensity (cm^{-1}) [b]	-	1483	3602	3456	4438	7419	12323	9021

[a] the band in the near UV region

[b] the band in the visible region