Ab Initio Investigation of Polyethylene Glycol (PEG) Coating of TiO_2 (101) Surfaces.

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SUPPORTING INFORMATION

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S.1 LOW COVERAGE

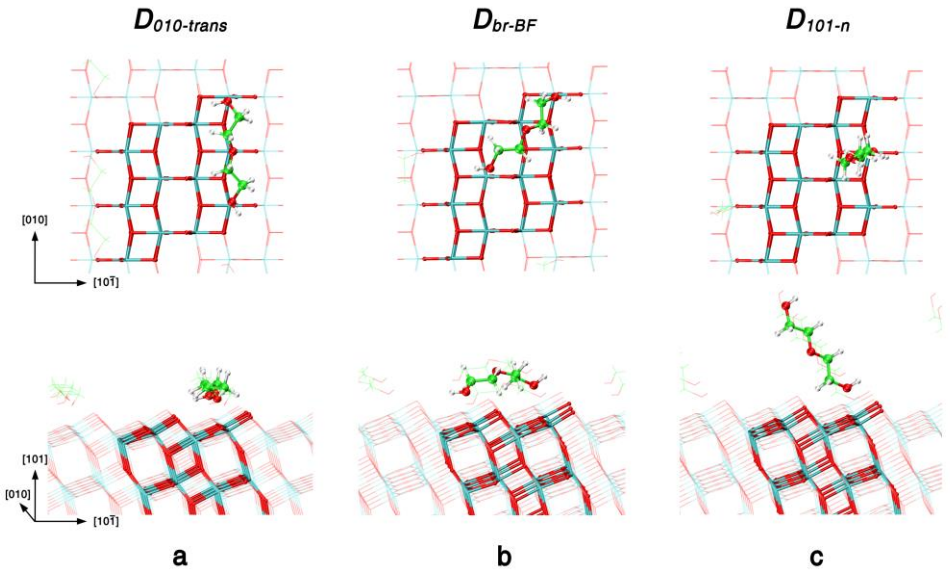

Figure 1S. Optimized structures of a) $D_{010\text{-}trans}$, b) $D_{br\text{-}BF}$ and c) $D_{101\text{-}n}$ PEG dimer molecule adsorption on the TiO_2 (101) anatase surface. These are the less stable configurations obtained in the low coverage regime. See Table 1S and Table 2.

Table 1S. Total adsorption energy and adsorption energy per site (expressed in eV) for molecular, mono- and bi-dissociated PEG dimer molecules adsorbed onto TiO_2 (101) anatase surface in the low coverage regime. This table integrates Table 2 in the main text. See Fig. 2, Fig 4, Fig. 2S and Fig. 3S for the corresponding equilibrium structures.

LOW COVERAGE									
	Molecular			*Monodissociated*			*Bidissociated*		
	Fig.	ΔE_{ads}	ΔE_{ads}^{site}	*Fig.*	ΔE_{ads}	ΔE_{ads}^{site}	*Fig.*	ΔE_{ads}	ΔE_{ads}^{site}
$D_{010\text{-}cis}$	2a	-1.88	-0.63	4a	-1.79	-0.60	3Sa	-1.68	-0.56
$D_{010\text{-}trans}$	1Sa	-1.82	-0.61	2Sa.1	-1.77	-0.59	3Sb	-1.68	-0.56
				2Sa.2	-1.74	-0.58			
$D_{br\text{-}AD}$	2b	-1.82	-0.91	2Sb.1	-1.94	-0.97	4b	-1.98	-0.99
				2Sb.2	-1.74	-0.87	3Sc	-1.19	-0.59
				2Sb.3	-1.50	-0.75			
				2Sb.4	-1.65	-0.82			
$D_{br\text{-}BF}$	1Sb	-1.23	-0.61	2Sc	-1.18	-0.59	3Sd	-1.18	-0.59
$D_{101\text{-}f}$	2c	-0.99	-0.99	4c	-0.78	-0.78		N.A.	N.A.
$D_{101\text{-}n}$	1Sc	-0.88	-0.88	2Sd	-0.74	-0.74		N.A.	N.A.

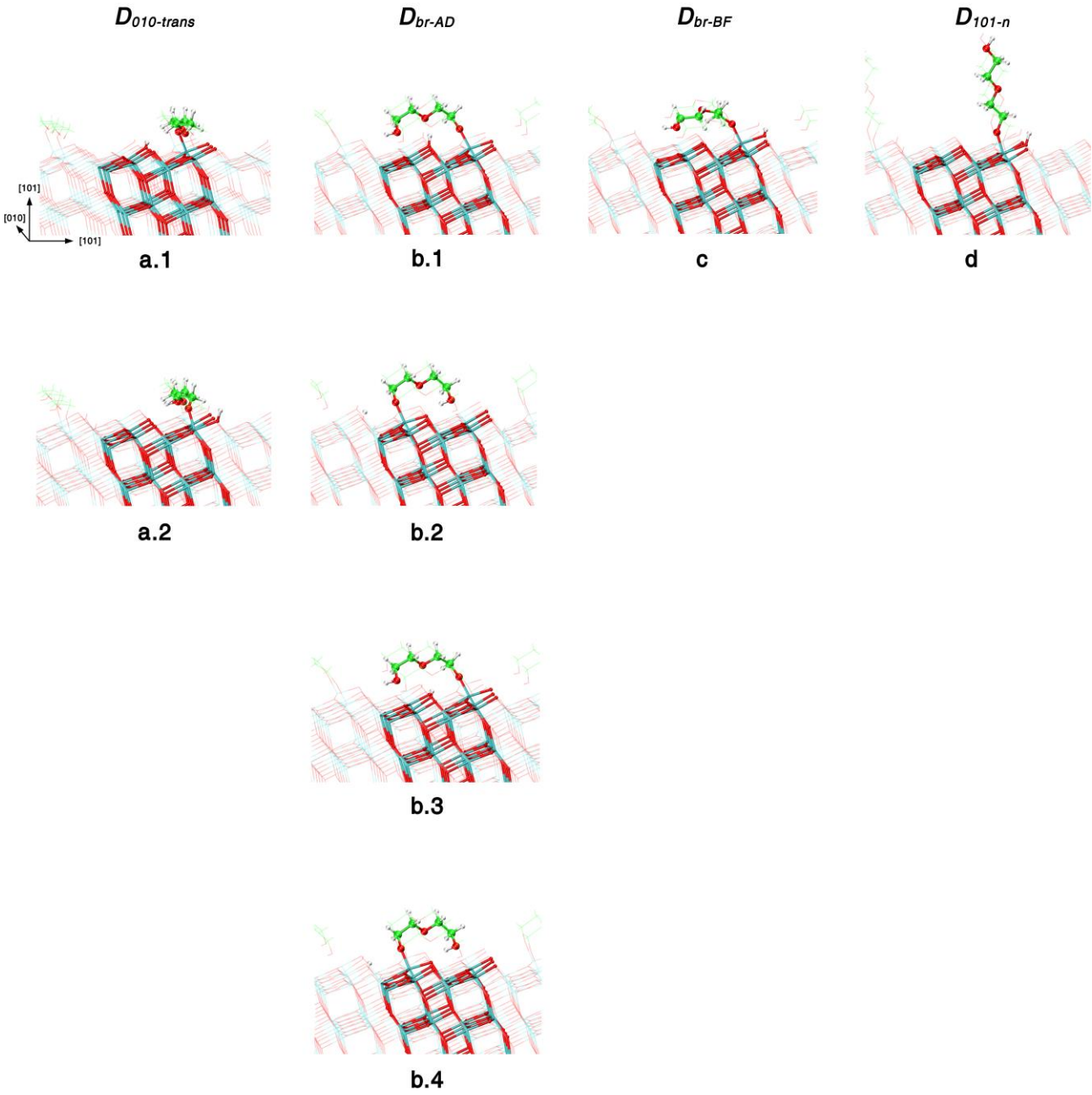

Figure 2S. Optimized structures of monodissociated PEG dimer molecule adsorption on the TiO_2 (101) anatase surface in the low coverage regime. See Table 1S and Table 2.

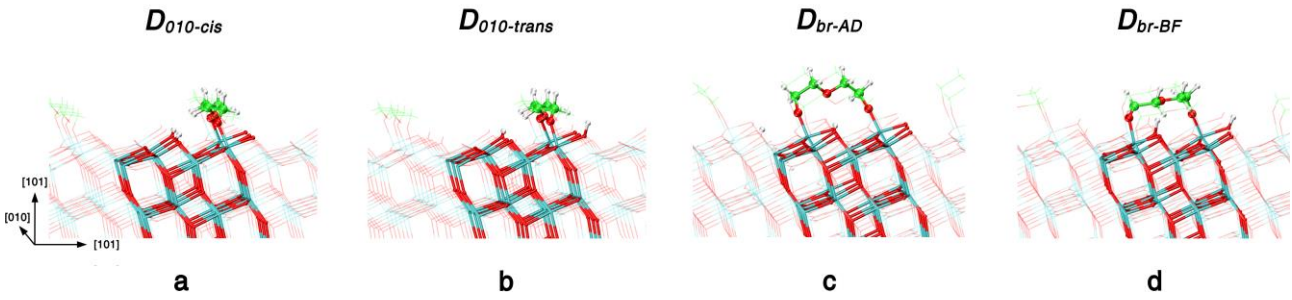

Figure 3S. Optimized structures of bidissociated PEG dimer molecule adsorption on the TiO_2 (101) anatase surface in the low coverage regime. See Table 1S and Table 2.

S.2 MEDIUM COVERAGE

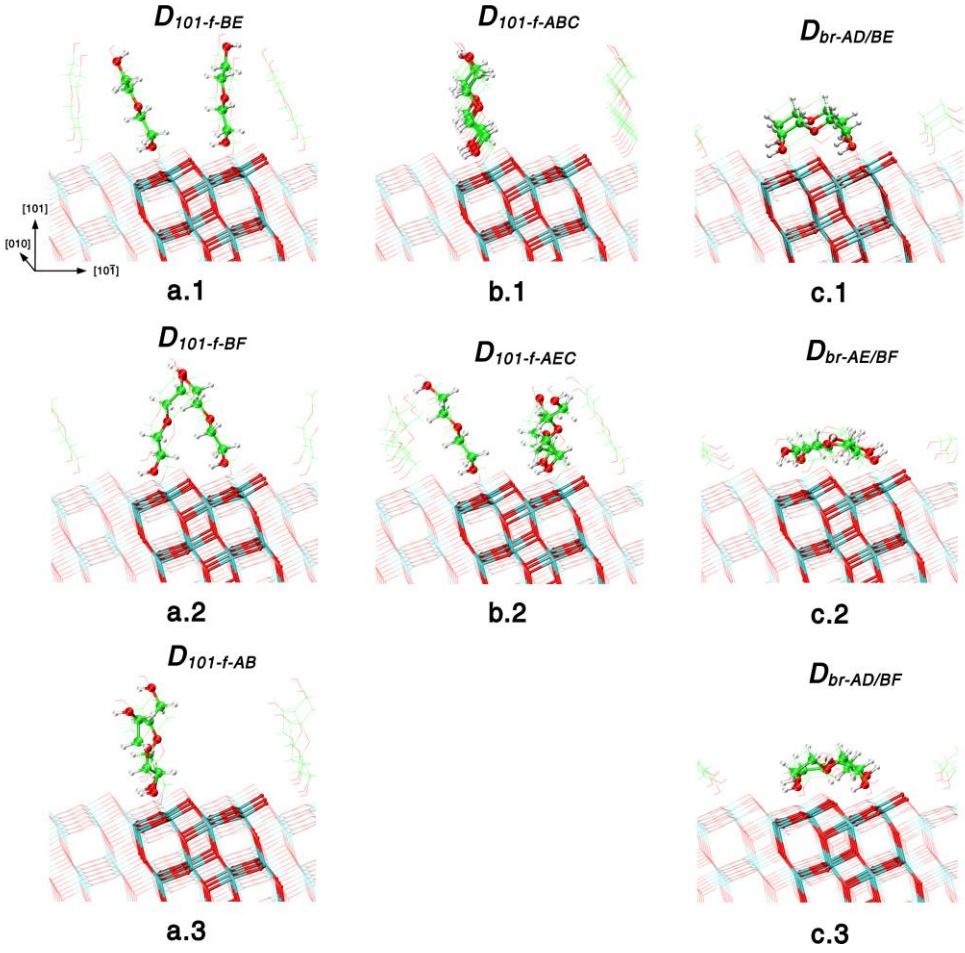

Figure 4S. Optimized structures of PEG dimer molecules adsorption on the TiO_2 (101) anatase surface in the medium coverage regime. See Table 3.

S.3 FULL COVERAGE

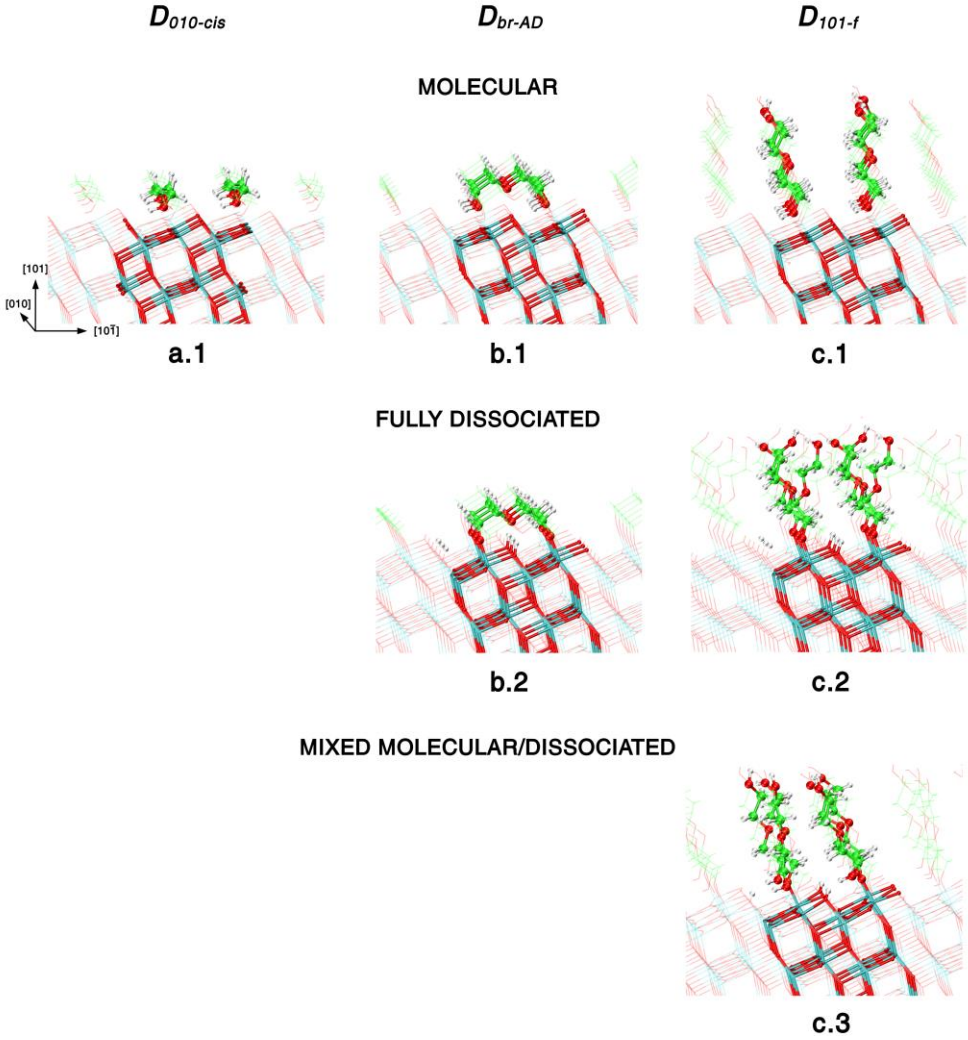

Figure 5S. Optimized structures of PEG dimer molecules adsorption on the TiO_2 (101) anatase surface in the full coverage regime. See Table 4.

S.4 WATER ADSORPTION

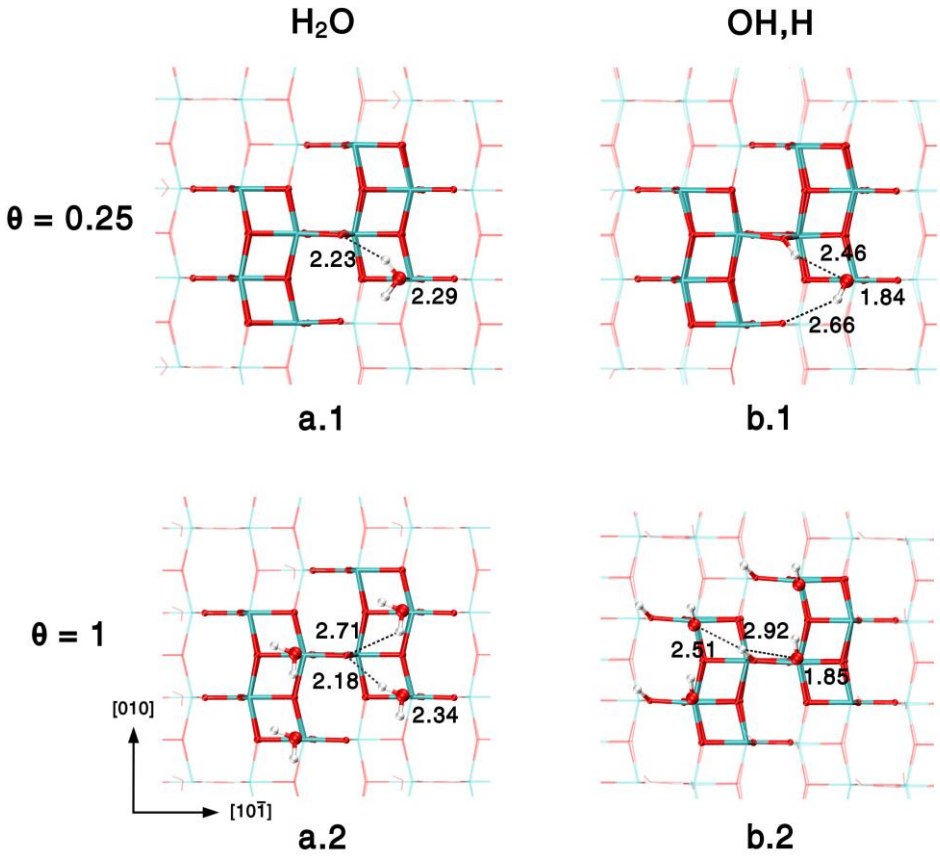

Figure 6S. Optimized structures of water adsorption on the TiO_2 (101) anatase surface, in the molecular (H_2O) and dissociated (OH,H) modes. Different level of coverage θ = 0.25 and θ =1 are considered.