

**Table S11: Atomistic nanodescriptors with sample values for 10 nm TiO<sub>2</sub>.**

	Descriptor name	TiO <sub>2</sub>
	Diameter (nm)	10
Chemical composition	Log of total No. of atoms in NP.	4,702146
	Log of total No. of atoms in core region of NP.	4,564702
	Log of total No. of atoms in surface region of NP.	4,135578
	Log of total No. of Me atoms in NP.	4,225025
	Log of total No. of Me atoms in core region of NP.	4,088172
	Log of total No. of Me atoms in surface region of NP.	3,656864
	Log of total No. of O atoms in NP.	4,526055
	Log of total No. of O atoms in surface region of NP.	3,96028
Potential Energy	Avg. pot. energy of all atoms in NP in eV.	-40,1659
	Avg. pot. energy of atoms in core region of NP in eV.	-40,5054
	Avg. pot. energy of atoms in surface region of NP in eV.	-39,254
	Relative avg. pot. energy of Me atoms in NP in eV.	-78,6862
	Relative avg. pot. energy of Me atoms in core region of NP in eV.	-79,3346
	Relative avg. pot. energy of Me atoms in surface region of NP in eV.	-76,9356
	Relative avg. pot. energy of O atoms in NP in eV.	-20,9057
	Relative avg. pot. energy of O atoms in surface region of NP in eV.	-41,0328
Topology	Avg. coordination No. of all atoms in NP.	3,882383
	Avg. coordination No. of atoms in core region of NP.	4,001362
	Avg. coordination No. of atoms in surface region of NP.	3,562793
	Avg. coordination No. of Me atoms in NP.	5,823575
	Avg. coordination No. of Me atoms in core region of NP.	6
	Avg. coordination No. of Me atoms in surface region of NP.	5,34729
	Avg. coordination No. of O atoms in NP.	2,911787
	Avg. coordination No. of O atoms in surface region of NP in.	2,675433
Size	Diameter of the NP in Å.	99,99438
	Surface area of the NP in Å <sup>2</sup> .	31412,37
	Volume of the NP in Å <sup>3</sup> .	523510
Lattice energy	Lattice energy of NP in eV.	-120,498
	Relative lattice energy of NP to bulk material (eV)	-0,93972
	Lattice energy of NP divided by the diameter of NP.	-1,20504
	Lattice energy of NP per unit surface area.	-0,00384
	Lattice energy of NP per unit volume.	-0,00023
Force vector	Avg. length of force vector for all atoms	1,449142
	Avg. length of force vector for all atoms in core region	0,488537
	Avg. length of force vector for all atoms in surface region	4,029433
	Avg. length of force vector for all Me atoms	1,411663
	Avg. length of force vector for Me atoms in core region	0,002976
	Avg. length of force vector for Me atoms in surface region	5,214622

Fo rce ve cto r	Avg. length of force vector for all O atoms	1,467881
	Avg. length of force vector for O atoms in core region	33,74856
	Avg. length of force vector for O atoms in surface region	47,59623
	Avg. length of force vector surface normal component for all atoms	-0,05728
	Avg. length of force vector surface normal component for all atoms in core region	-0,0008
	Avg. length of force vector surface normal component for all atoms in surface region	-0,209
	Avg. length of force vector surface normal component for all Me atoms	-0,42259
	Avg. length of force vector surface normal component for Me atoms in core region	0,000104
	Avg. length of force vector surface normal component for Me atoms in surface region	-1,56372
	Avg. length of force vector surface normal component for all O atoms	0,125376
	Avg. length of force vector surface normal component for O atoms in core region	0,731813
	Avg. length of force vector surface normal component for O atoms in surface region	3,440085
	Avg. length of force vector surface tangent component for all atoms	0,993472
	Avg. length of force vector surface tangent component for all atoms in core region	0,382975
	Avg. length of force vector surface tangent component for all atoms in surface region	2,633335
	Avg. length of force vector surface tangent component for all Me atoms	0,812424
	Avg. length of force vector surface tangent component for Me atoms in core region	0,000887
	Avg. length of force vector surface tangent component for Me atoms in surface region	3,003286
	Avg. length of force vector surface tangent component for all O atoms	1,083997
	Avg. length of force vector surface tangent component for O atoms in core region	-0,00125
Avg. length of force vector surface tangent component for O atoms in surface region	0,464644	