

Effect of Size and Structure on the Ground and Excited State

Electronic Structure of TiO₂ Nanoparticles

DaeheumCho,^a KyoungChulKo,^{ab} Oriol Lamiel-García,^b Stefan T. Bromley,^{bc} Jin Yong Lee^{a*} and Francesc Illas^{b*}

^{a)} *Department of Chemistry, Sungkyunkwan University, Suwon 16419, Korea*

^{b)} *Departament de Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franquès 1, 08028 Barcelona, Spain*

^{c)} *Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain*

* Corresponding authors: jinylee@skku.edu (J. Y. Lee), francesc.illas@ub.edu (F. Illas)

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1. Comparison between $(S_0 \rightarrow S_1)_v$ and $(S_0 \rightarrow T_1)_v$ excitations.

Table S1. $(S_0 \rightarrow S_1)_v$ and $(S_0 \rightarrow T_1)_v$ excitation energies (in eV) calculated at B3LYP/6-31G(d)/Vacuum, Δ corresponds to the $(S_0 \rightarrow S_1)_v - (S_0 \rightarrow T_1)_v$ values.

# TiO2 units	4				8				16				35		84t
	a	b	c	d	a	b	c	d	a	b	c	d	G09-opt	AIMS	AIMS
$(S_0 \rightarrow S_1)_v$	3.93	3.56	2.41	3.80	4.11	3.85	3.87	3.79	3.61	4.08	4.13	2.37	3.67	3.36	3.40
$(S_0 \rightarrow T_1)_v$	3.87	3.52	2.37	3.72	4.03	3.80	3.79	3.73	3.58	4.02	4.03	2.36	3.64	3.34	3.38
Δ	0.06	0.04	0.04	0.08	0.09	0.05	0.08	0.06	0.03	0.06	0.10	0.00	0.03	0.02	0.02

Table S2. $(S_0 \rightarrow S_1)_v$ and $(S_0 \rightarrow T_1)_v$ excitation energies (in eV) calculated at CAM-B3LYP/6-31G(d)/Vacuum, Δ corresponds to the $(S_0 \rightarrow S_1)_v - (S_0 \rightarrow T_1)_v$ values.

# TiO2 units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
$(S_0 \rightarrow S_1)_v$	4.41	4.04	3.82	4.22	4.75	4.79	4.35	4.72	4.74	4.90	4.65	4.24	4.52	3.88	4.17
$(S_0 \rightarrow T_1)_v$	4.32	3.98	3.76	4.13	4.55	4.53	4.25	4.43	4.57	4.67	4.51	4.11	4.39	4.05	-
Δ	0.09	0.06	0.06	0.09	0.2	0.26	0.1	0.29	0.17	0.23	0.14	0.13	0.13	-0.17	-

2. Energy per unit of the (TiO₂)_n particles with n = 4, 8, 16, 35 and 84 as predicted from B3LYP/6-31G(d)/Water.

Table S3. Energy / TiO₂ units (E_{unit/84}) relative to that of 84 unit at B3LYP/6-31G(d)/Water.

# TiO ₂ units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
E _{unit/84}	1.15	1.22	1.00	1.04	0.51	0.56	0.60	0.64	0.19	0.21	0.26	0.32	0.20	0.22	0.00

3. E_{gap} , O_{gap} , and $\Delta E_{\text{H-L}}$ (in eV) obtained at different level of theories.Table S4. E_{gap} , O_{gap} , and $\Delta E_{\text{H-L}}$ (in eV) obtained at B3LYP/6-31G(d)/Vacuum level

# TiO ₂ units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
E_{gap}	8.72	8.28	6.44	7.84	7.80	7.37	7.50	7.37	6.75	7.00	7.40	5.43	6.13	5.78	5.31
O_{gap}	3.93	3.56	2.41	3.80	4.11	3.85	3.87	3.79	3.61	4.08	4.13	2.37	3.67	3.36	3.40
$\Delta E_{\text{H-L}}$	5.08	4.72	3.06	4.65	4.88	4.48	4.57	4.46	4.18	4.75	5.05	2.75	4.41	4.07	4.02

Table S5. E_{gap} , O_{gap} , and $\Delta E_{\text{H-L}}$ (in eV) obtained at B3LYP/6-31G(d)/Water level

# TiO ₂ units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
E_{gap}	5.23	4.84	4.62	5.63	5.00	4.83	4.82	4.85	4.32	5.05	5.07	3.72	4.08	3.80	3.74
O_{gap}	4.26	3.88	4.31	4.59	4.28	4.34	4.12	4.31	4.05	4.32	4.24	3.61	3.69	3.43	3.43
$\Delta E_{\text{H-L}}$	5.49	5.09	5.04	5.80	5.32	5.18	5.22	5.20	4.77	5.27	5.11	4.11	4.45	4.15	4.07

Table S6. E_{gap} , O_{gap} , and $\Delta E_{\text{H-L}}$ (in eV) obtained at CAM-B3LYP/6-31G(d)/Vacuum level.

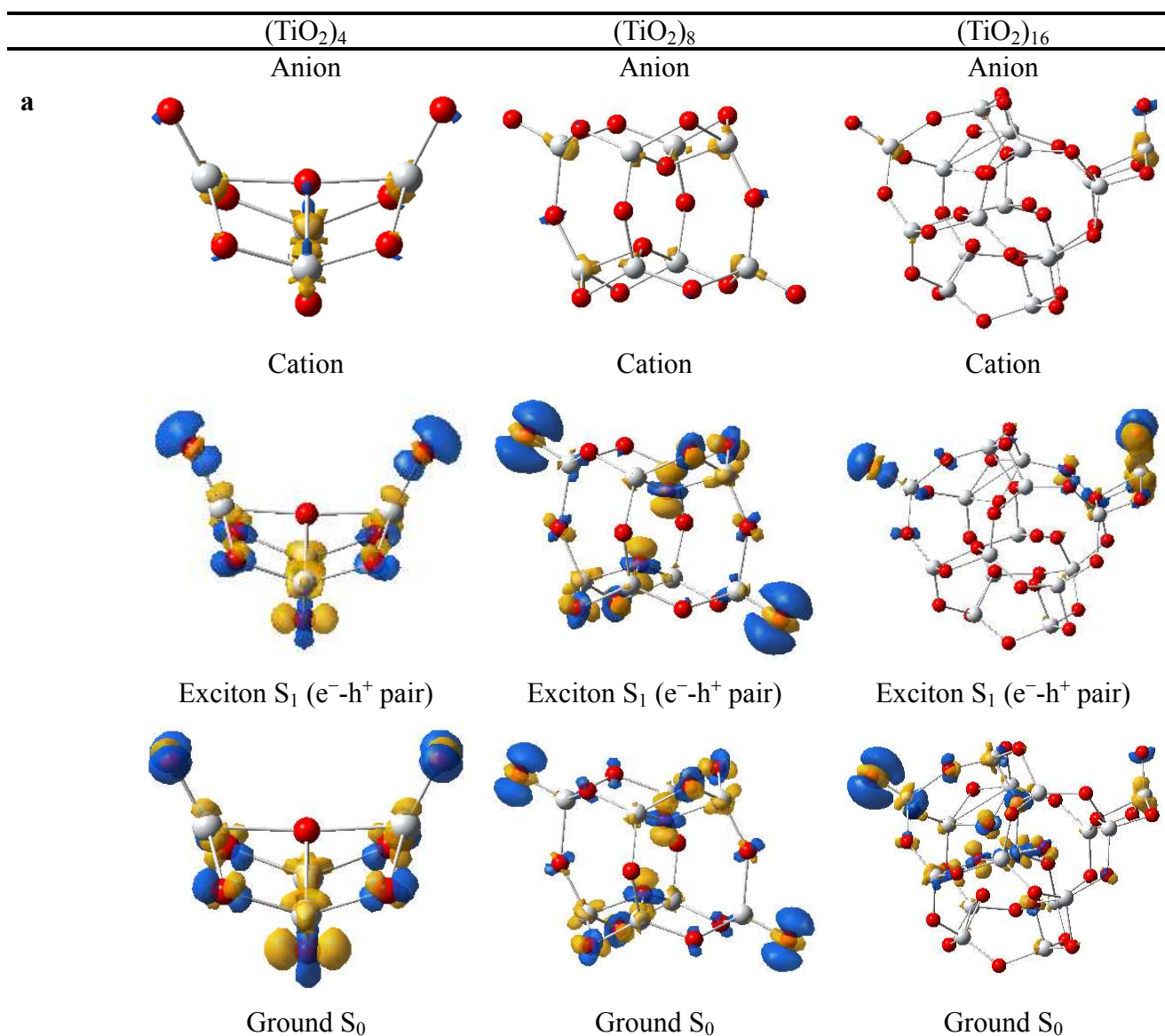
# TiO ₂ units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
E_{gap}	9.47	8.96	7.04	8.81	8.99	8.43	8.01	8.19	7.20	8.44	8.56	6.19	7.26	6.68	6.53
O_{gap}	4.41	4.04	3.82	4.22	4.75	4.79	4.35	4.72	4.74	4.90	4.65	4.24	4.52	3.89	4.17
$\Delta E_{\text{H-L}}$	8.33	7.89	5.97	7.65	8.08	7.67	7.73	7.61	7.34	7.89	8.06	5.85	7.36	6.88	6.82

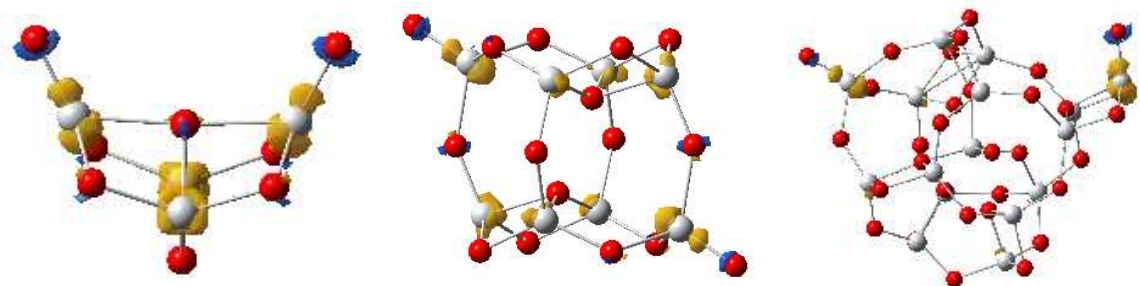
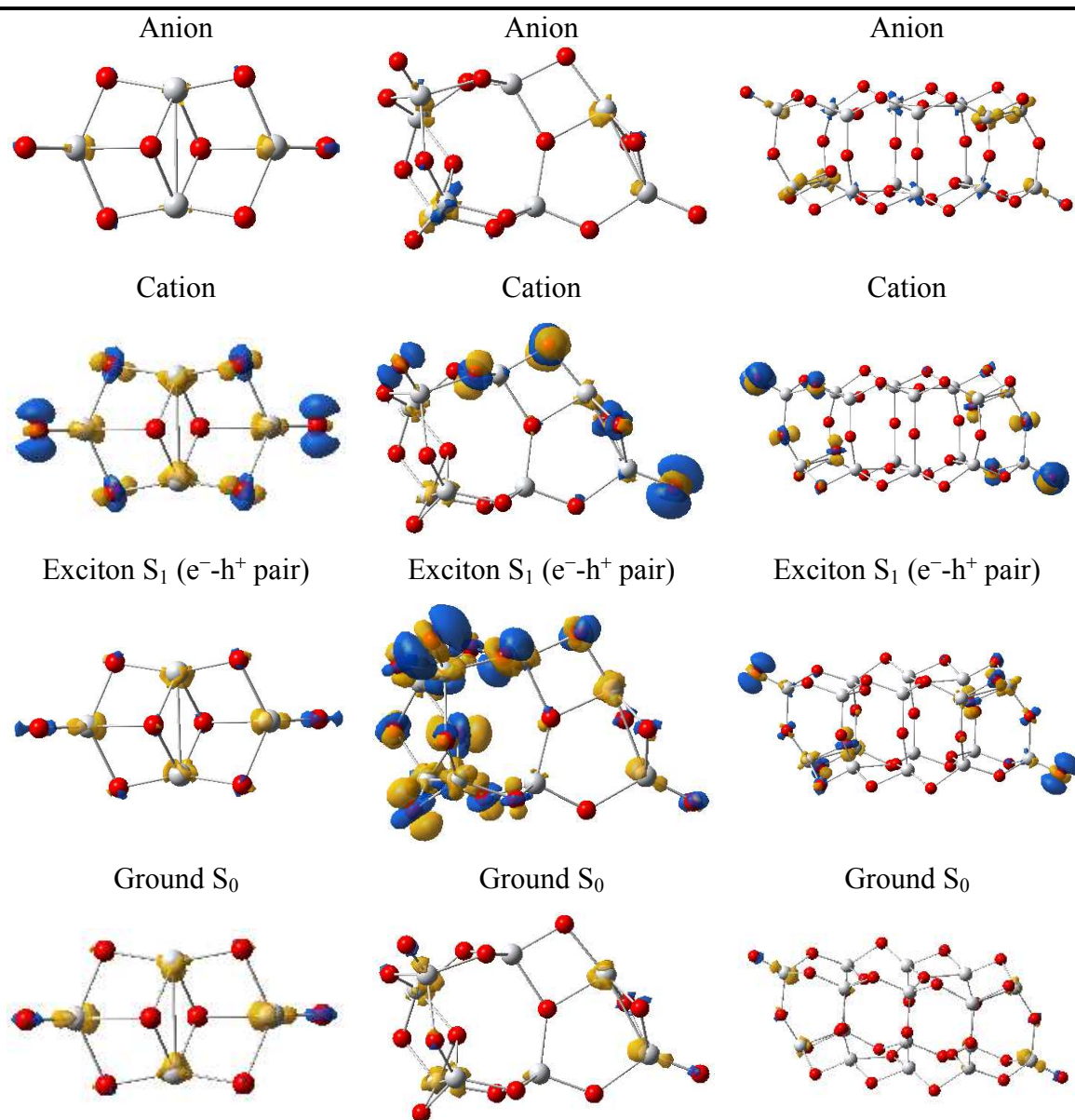
Table S7. E_{gap} , O_{gap} , and $\Delta E_{\text{H-L}}$ (in eV) obtained at CAM-B3LYP/6-31G(d)/Water level

# TiO ₂ units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
E_{gap}	5.93	5.43	5.21	6.61	6.31	5.73	5.65	5.52	4.71	6.13	5.95	4.38	5.08	4.61	5.86
O_{gap}	4.72	4.35	4.82	5.05	4.84	4.88	4.61	4.87	4.77	4.95	4.88	4.33	4.54	4.21	4.19
$\Delta E_{\text{H-L}}$	8.69	8.26	8.14	8.88	8.41	8.32	8.31	8.33	7.86	8.26	8.12	7.20	7.36	6.97	6.87

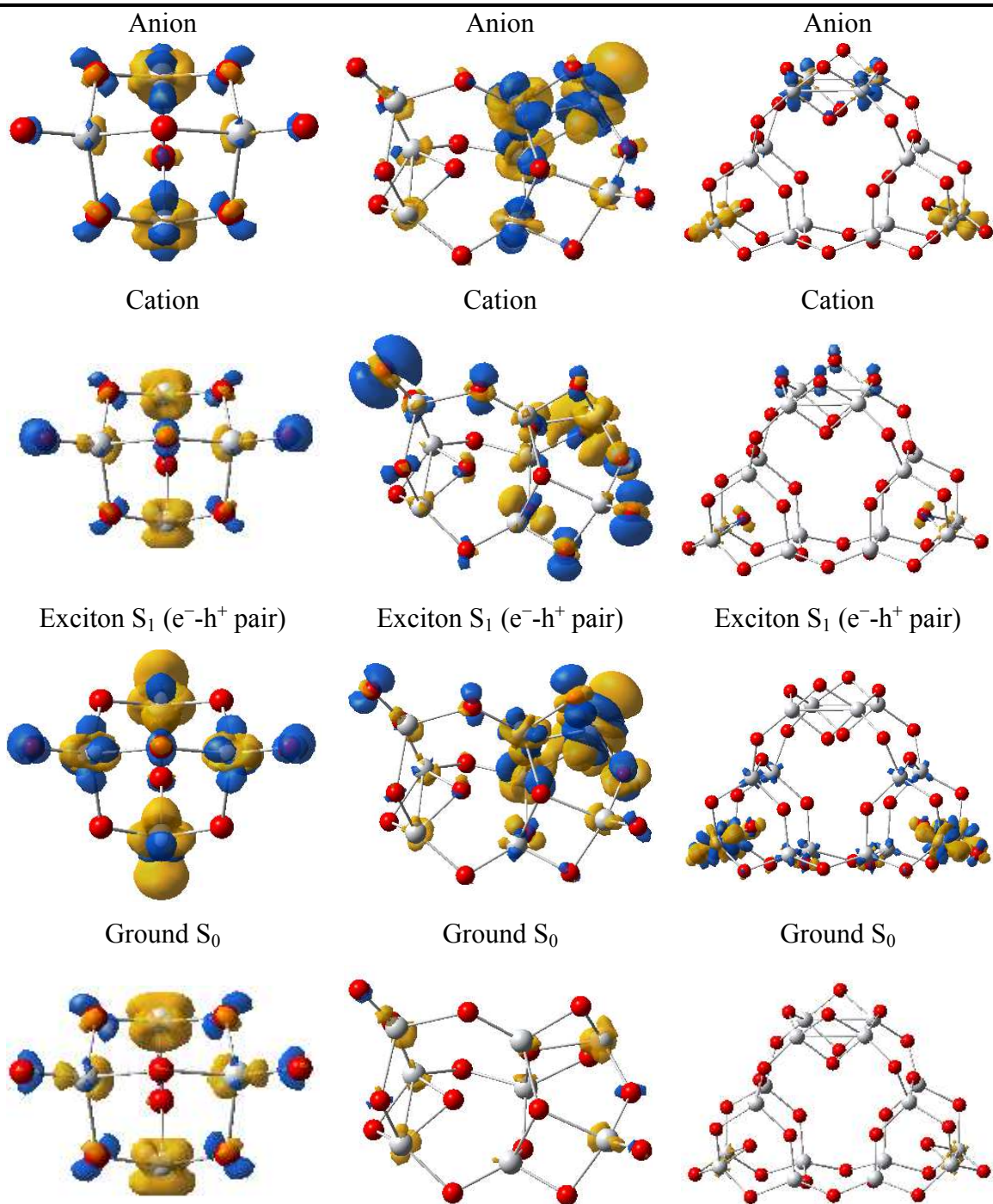
4. Neutralization of unique charge localization patterns of each isomer upon water solvation.

Figure S1. Difference of charge density (isovalue = $0.004 \text{ e}^-/\text{\AA}^3$) illustrating electron redistribution of TiO_2 in vertically generated anion, cation, S_1 exciton, and ground states upon water solvation at B3LYP/6-31G(d) level. Blue: electron gain; Red: electron lose. The maps below show that electron density moves from the most negative Ti^{3+} to the most positive O^{2-} , resulting in a more equal distribution of electrons on each atomic species (e.g. Ti^{3+} or O^{2-}).

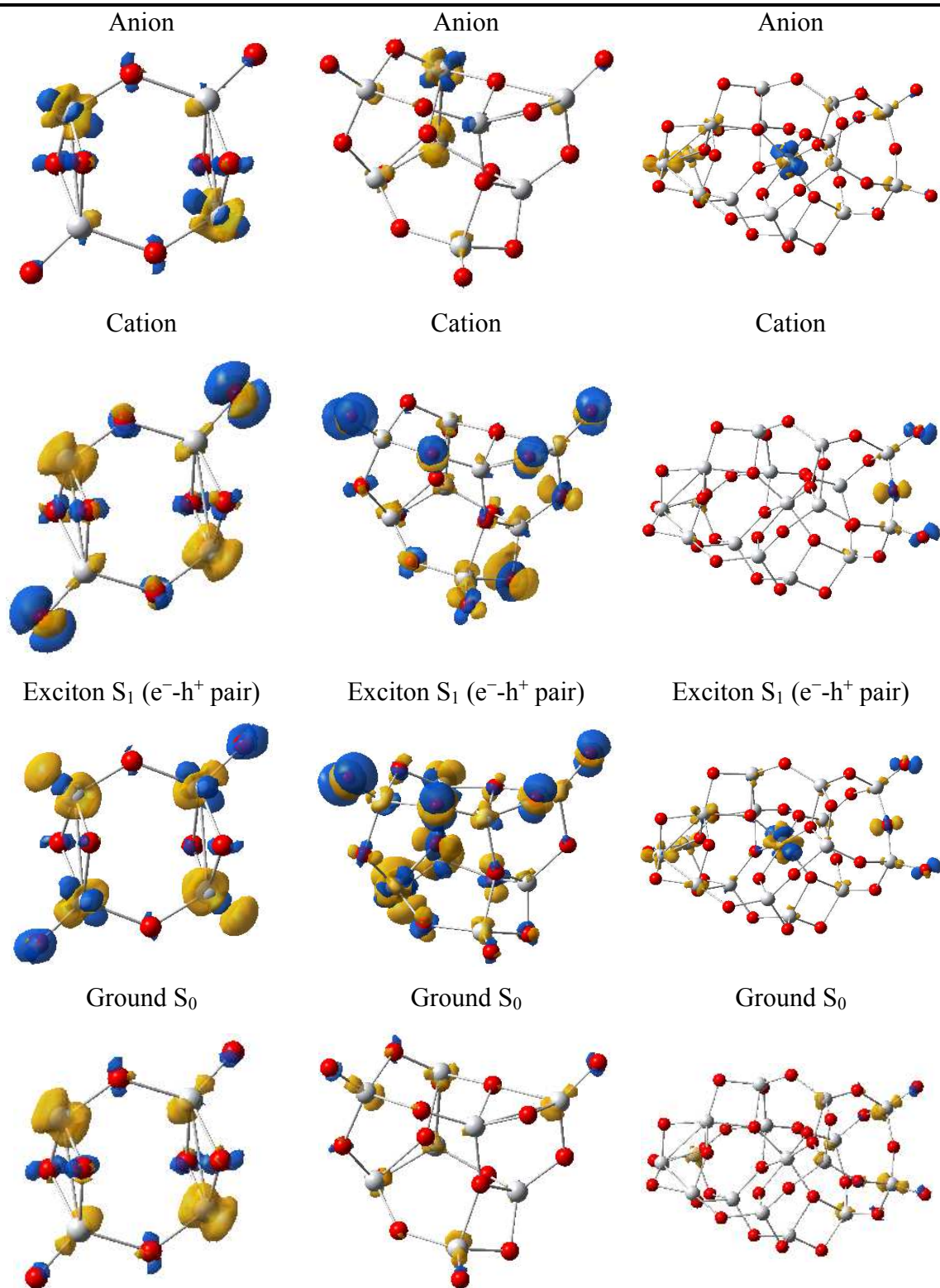


**b**

c



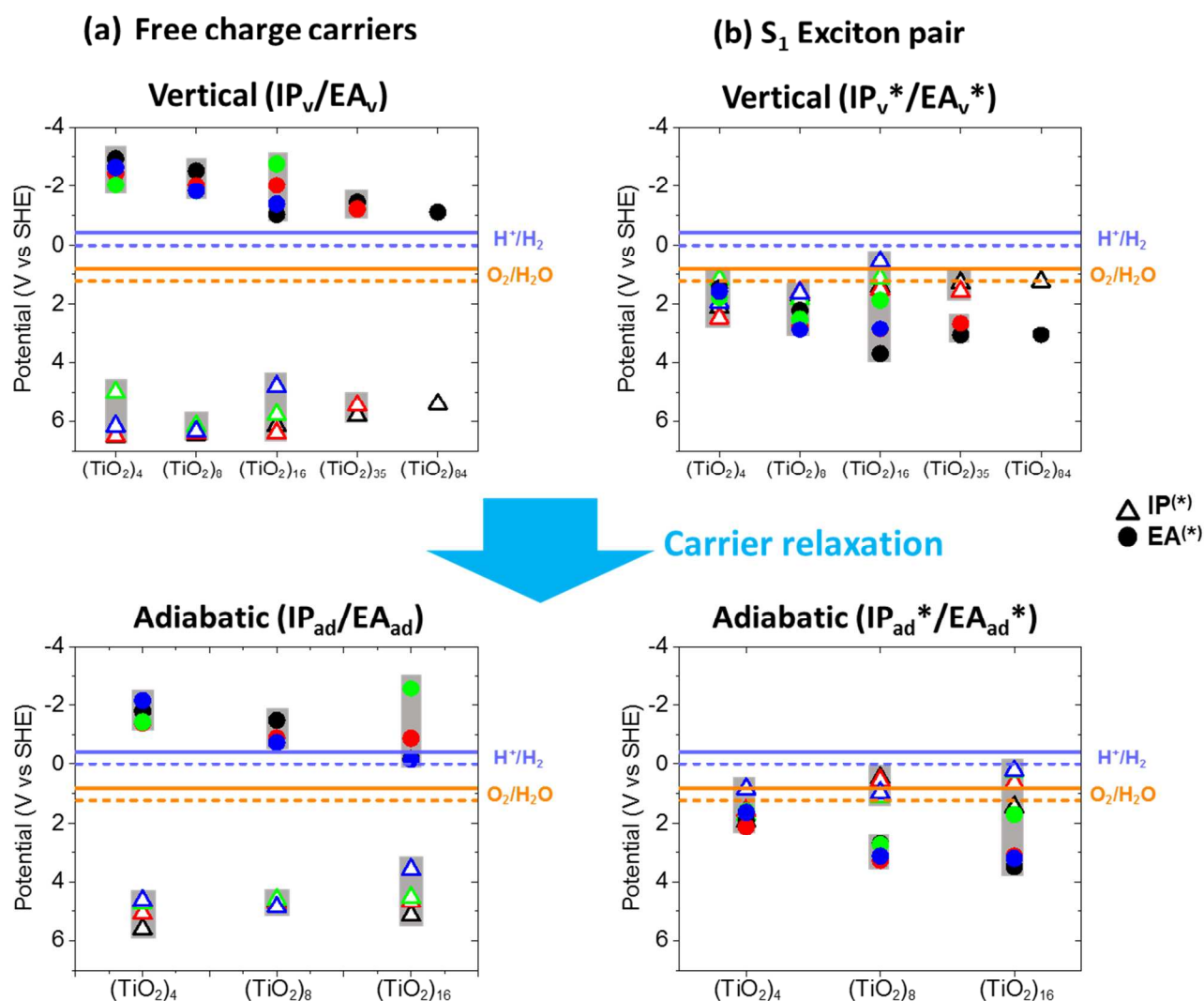
d



5. Water splitting capabilities of TiO₂ NPs (IP/EA and IP*/EA* diagram) obtained at CAM-B3LYP/6-31G(d) level.

Figure S2. Calculated vertical (top panel) and adiabatic (bottom panel) IP (triangle), EA (circle) of the TiO₂ nanoparticle free charge carrier (left) and S₁ exciton states (right) in vacuum, relative to absolute value of the experimental SHE potential (4.44 eV) at CAM-B3LYP/6-31G(d) level. Potentials for HER (violet lines) and OER (orange lines) at pH = 0 (dashed lines) and pH = 7 (solid lines) are shown. Thermodynamically more stable state between free charge carrier and S₁ exciton in vertical and adiabatic time scale are marked in green. Color codes: Black for isomer a (tentative global minimum), red for isomer b, green for isomer c, and blue for isomer d.

CAM-B3LYP / Vacuum



Water splitting ability of TiO_2 nanoparticles in vacuum. The left panel of Figure S2, clearly shows that, in vacuum, all vertical and adiabatic IP related processes favor OER because standard reduction potentials of the IP reactions are located in the 3-5 V region which is higher (more positive) than experimental OER potential (1.23 V at pH = 0). Furthermore, all of the nanoparticles also have thermodynamic driving force for the HER reaction (0.0 V in pH = 0) driven by EA related processes, except $(\text{TiO}_2)_{16a,16d}$, although the reactions are slightly less exothermic than in the case of IP related processes.

Let us now consider the situation for the exciton state which, for the nanoparticles, is always more stable than the free carrier state in vacuum. In other words, the $\text{IP}_v^*/\text{EA}_v^*$ defining the potentials for the exciton are the relevant quantities for finite nanoparticles since it involves the real excited state rather than the metastable free charge carriers. Compared to corresponding IP_v/EA_v related standard reductions potentials, these values are more negative/positive by the amount of the O_{gap} excitation energy. As a consequence, both IP_v^* and EA_v^* potentials in vacuum are located in close proximity energetically, spanning 0-3 V regions. This is higher than the potential of the HER half-reaction as clearly shown in the left panel of Figure 7b. Therefore, in vacuum, none of the TiO_2 nanoparticles explored facilitates the HER reaction simply because all of the IP_v^* and EA_v^* potentials are located in a region above HER potential. Interestingly, most of the nanoparticles in vacuum can still drive the OER reaction.

The same discussions can apply to adiabatic $\text{IP}^{(*)}/\text{EA}^{(*)}$ cases (Figure S2 bottom panel), excepting the lowering/lifting of IP/EA in the free charge carriers and lifting/lowering of IP^*/EA^* in the S_1 exciton due to geometry relaxation in the excited state. In conclusion, TiO_2 nanoparticles are incapable of facilitating photocatalytic only free charge carriers

Figure S3. Calculated vertical (top panel) and adiabatic (bottom panel) IP (triangle), EA (circle) of the TiO_2 nanoparticle free charge carrier (left) and S_1 exciton states (right) in water, relative to absolute value of the experimental SHE potential (4.44 eV) at B3LYP/6-31G(d) level. Potentials for HER (violet lines) and OER (orange lines) at pH = 0 (dashed lines) and pH = 7 (solid lines) are shown. Thermodynamically more stable state between free charge carrier and S_1 exciton in vertical and adiabatic time scale are marked in green. Color codes: Black for isomer a (tentative global minimum), red for isomer b, green for isomer c, and blue for isomer d. Note that B3LYP calculations at the S_1 excited state failed (see explanation in main text).

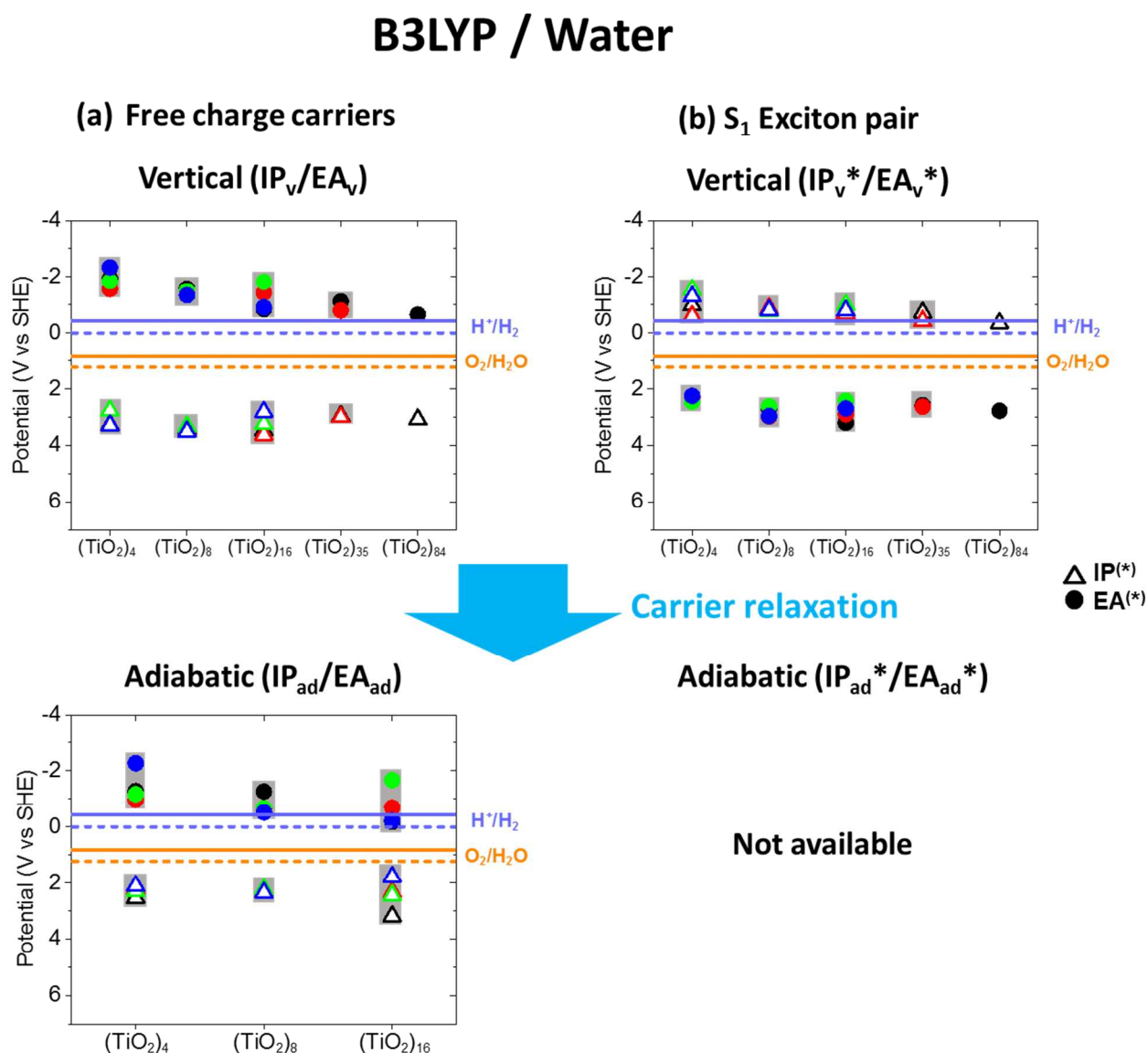
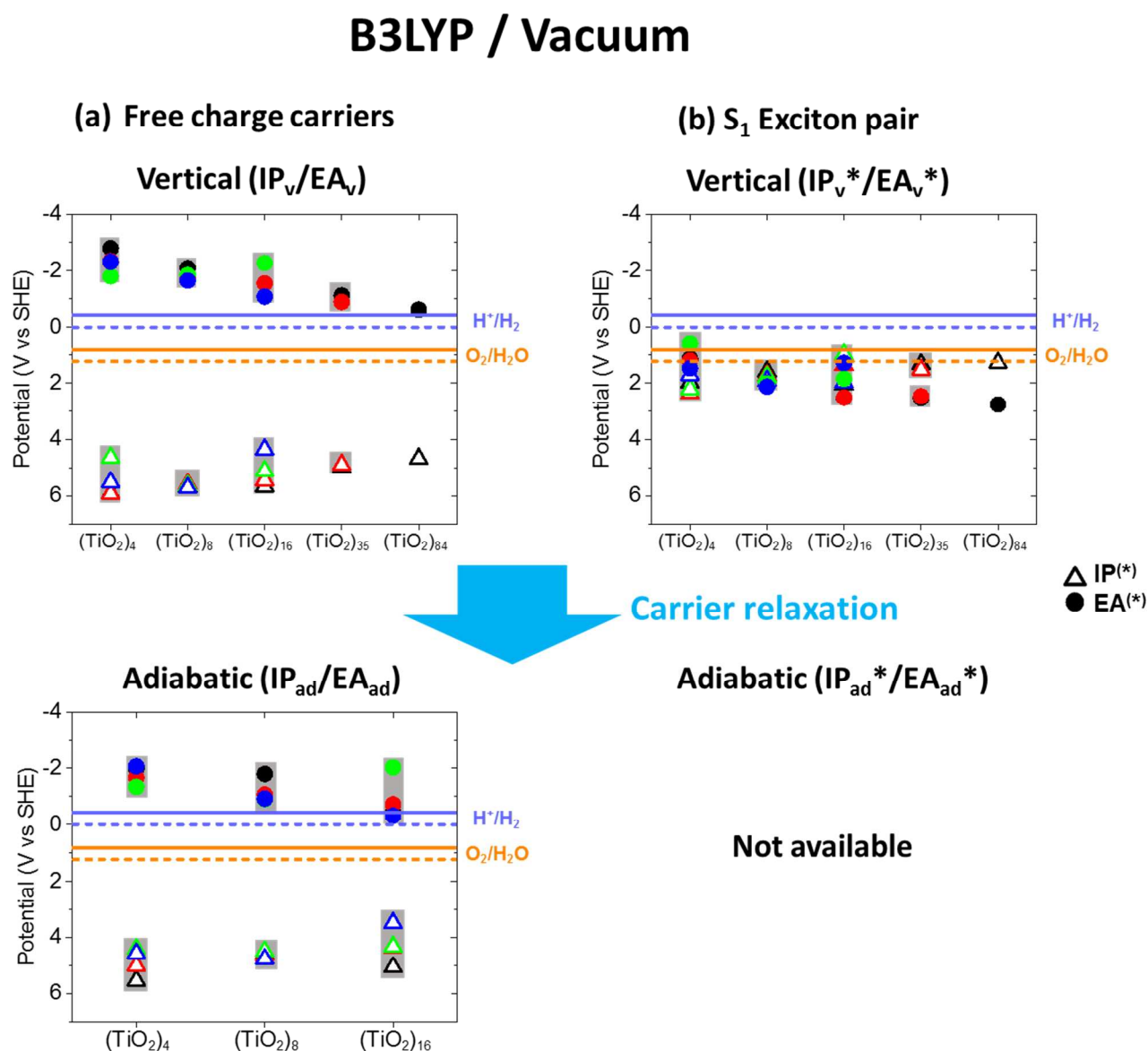


Figure S4. Calculated vertical (top panel) and adiabatic (bottom panel) IP (triangle), EA (circle) of the TiO_2 nanoparticle free charge carrier (left) and S_1 exciton states (right) in vacuum, relative to absolute value of the experimental SHE potential (4.44 eV) at B3LYP/6-31G(d) level. Potentials for HER (violet lines) and OER (orange lines) at pH = 0 (dashed lines) and pH = 7 (solid lines) are shown. Thermodynamically more stable state between free charge carrier and S_1 exciton in vertical and adiabatic time scale are marked in green. Color codes: Black for isomer a (tentative global minimum), red for isomer b, green for isomer c, and blue for isomer d. Note that B3LYP calculations at the S_1 excited state failed (see explanation in main text).



5.1. Vertical and adiabatic $IP^{(*)}/EA^{(*)}$ potentials relative to vacuum energy level (not relative to SHE potential).

Table S8. Vertical and adiabatic $IP^{(*)}/EA^{(*)}$ potentials of the TiO_2 nanoparticles in vacuum calculated at CAM-B3LYP/6-31G(d) level.

# TiO_2 units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
IP_v	11.0	10.9	9.4	10.6	10.9	10.8	10.6	10.8	10.6	10.8	10.2	9.2	10.3	9.9	9.9
EA_v	1.5	2.0	2.4	1.8	1.9	2.4	2.6	2.6	3.4	2.4	1.7	3.0	3.0	3.2	3.3
IP_{ad}	10.1	9.5	9.2	9.1	9.1	9.2	9.0	9.3	9.6	9.1	9.0	8.0	-	-	-
EA_{ad}	2.6	3.0	3.0	2.3	3.0	3.5	3.7	3.7	4.2	3.6	1.9	4.3	-	-	-
IP_v^*	6.6	6.9	5.6	6.4	6.1	6.1	6.3	6.1	5.9	5.9	5.6	5.0	5.7	6.0	5.7
EA_v^*	5.9	6.0	6.2	6.0	6.7	7.2	7.0	7.3	8.1	7.3	6.3	7.3	7.5	7.1	7.5
IP_{ad}^*	6.4	6.0	6.2	5.3	4.9	5.0	5.5	5.4	5.9	5.1	4.7	4.7	-	-	-
EA_{ad}^*	6.3	6.6	6.0	6.1	7.2	7.7	7.2	7.6	7.9	7.6	6.1	7.7	-	-	-

Table S9. Vertical and adiabatic $IP^{(*)}/EA^{(*)}$ potentials of the TiO_2 nanoparticles in water calculated at CAM-B3LYP/6-31G(d) level.^a

# TiO_2 units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
IP_v	8.3	8.2	7.6	8.4	8.7	8.6	8.5	8.5	8.4	8.8	8.2	7.6	8.1	8.0	9.2
EA_v	2.4	2.8	2.4	1.8	2.4	2.9	2.9	3.0	3.7	2.7	2.2	3.2	3.0	3.4	3.3
IP_{ad}	7.0	6.7	7.1	6.6	6.8	6.8	6.8	6.9	7.7	7.0	7.1	6.3	-	-	-
EA_{ad}	3.5	3.9	3.2	2.0	3.6	4.0	3.9	4.1	4.5	3.9	2.2	4.4	-	-	-
IP_v^*	3.6	3.9	2.8	3.4	3.9	3.8	3.9	3.6	3.6	3.9	3.3	3.3	3.6	3.8	5.0
EA_v^*	7.1	7.1	7.2	6.9	7.3	7.8	7.5	7.8	8.4	7.6	7.1	7.6	7.6	7.6	7.5
IP_{ad}^*	3.0	3.0	2.5	2.1	2.4	2.5	2.7	2.8	4.0	2.9	2.6	2.6	-	-	-
EA_{ad}^*	7.5	7.7	7.7	6.5	8.0	8.4	8.0	8.1	8.2	7.9	6.7	8.1	-	-	-

^a Corresponding potentials (in eV) of hydrated $(TiO_2)_{23}$ rutile nanocrystal taken from Ref 64.: IP_v (7.92);

EA_v (3.44); IP_{ad} (5.75); EA_{ad} (4.52); IP_v^* (3.92); EA_v^* (7.40); IP_{ad} (2.45); EA_{ad} (3.82)

Table S10. Vertical and adiabatic IP^(*)/EA^(*) potentials of the TiO₂ nanoparticles in vacuum calculated at B3LYP/6-31G(d) level.

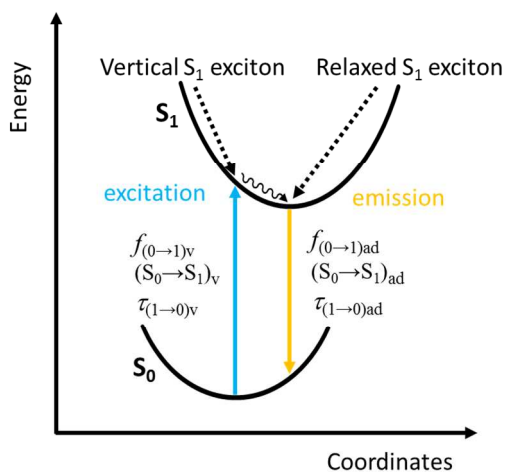
# TiO ₂ units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
IP _v	10.4	10.4	9.1	10.0	10.1	10.0	10.1	10.2	10.1	9.9	9.6	8.8	9.4	9.3	9.1
EA _v	1.6	2.1	2.6	2.1	2.3	2.7	2.6	2.8	3.4	2.9	2.2	3.4	3.3	3.6	3.8
IP _{ad}	10.0	9.5	8.9	9.0	9.0	9.1	8.9	9.2	9.5	8.8	8.8	7.9	-	-	-
EA _{ad}	2.5	2.8	3.1	2.4	2.6	3.4	3.5	3.5	4.0	3.7	2.4	4.1	-	-	-
IP _v [*]	6.4	6.8	6.7	6.2	6.0	6.2	6.2	6.4	6.5	5.8	5.4	6.4	5.8	6.0	5.7
EA _v [*]	5.6	5.6	5.0	5.9	6.5	6.5	6.5	6.6	7.0	7.0	6.3	5.7	7.0	6.9	7.2
IP _{ad} [*]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
EA _{ad} [*]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S11. Vertical and adiabatic IP^(*)/EA^(*) potentials of the TiO₂ nanoparticles in water calculated at B3LYP/6-31G(d) level.

# TiO ₂ units	4				8				16				35		84
	a	b	c	d	a	b	c	d	a	b	c	d	a	b	a
IP _v	7.7	7.7	7.2	7.7	7.9	7.9	7.8	7.9	7.9	8.1	7.7	7.3	7.4	7.4	7.5
EA _v	2.5	2.9	2.6	2.1	2.9	3.1	3.0	3.1	3.6	3.0	2.6	3.5	3.3	3.6	3.8
IP _{ad}	7.0	6.7	6.7	6.6	6.7	6.8	6.7	6.8	7.6	6.8	6.9	6.2	-	-	-
EA _{ad}	3.2	3.5	3.3	2.2	3.2	3.8	3.8	3.9	4.3	3.8	2.8	4.2	-	-	-
IP _v [*]	3.5	3.8	2.9	3.1	3.6	3.6	3.7	3.6	3.9	3.7	3.4	3.6	3.7	4.0	4.1
EA _v [*]	6.7	6.8	6.9	6.7	7.1	7.4	7.1	7.4	7.6	7.3	6.9	7.1	7.0	7.1	7.2
IP _{ad} [*]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
EA _{ad} [*]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

6. Excited state lifetime (τ) for vertical and relaxed S_1 excitons in vacuum and water.

Figure S5. Schematics for excited state lifetimes (radiative decay, $\tau_{(1 \rightarrow 0)}$) of vertical and relaxed (self-trapped) S_1 exciton and oscillator strength (f), excitation energy ($S_0 \rightarrow S_1$).



Excited state lifetime for vertical and relaxed S_1 exciton was calculated from the relationship between oscillator strength ($f_{(0 \rightarrow 1)}$), excitation energy ($S_0 \rightarrow S_1$) and Einstein's coefficient A_{ij} .

$$\tau_{(1 \rightarrow 0)} = \frac{1}{A_{10}} = \frac{2\pi\epsilon_0 m_e c^3}{n\omega^2 e^2 f_{(1 \rightarrow 0)}}$$

where n and ω are a refractive index of the medium and transition frequency ($\hbar\omega = (S_0 \rightarrow S_1)$).

Figure S6. Excited state lifetime (τ) for the vertical (filled circle) and relaxed (hollow triangle) S_1 exciton in (a) vacuum and (b) water calculated by CAM-B3LYP/6-31G(d) level.

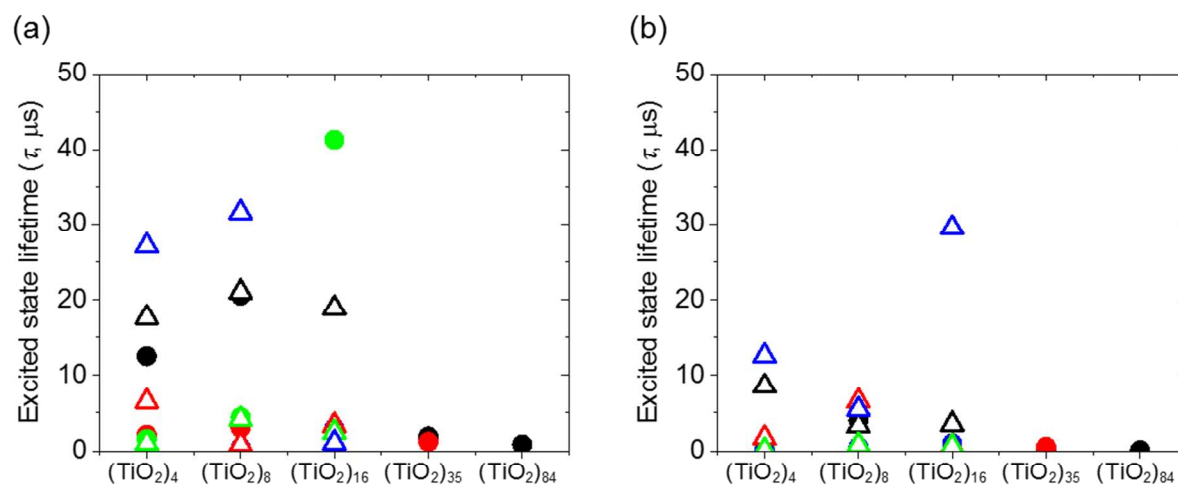
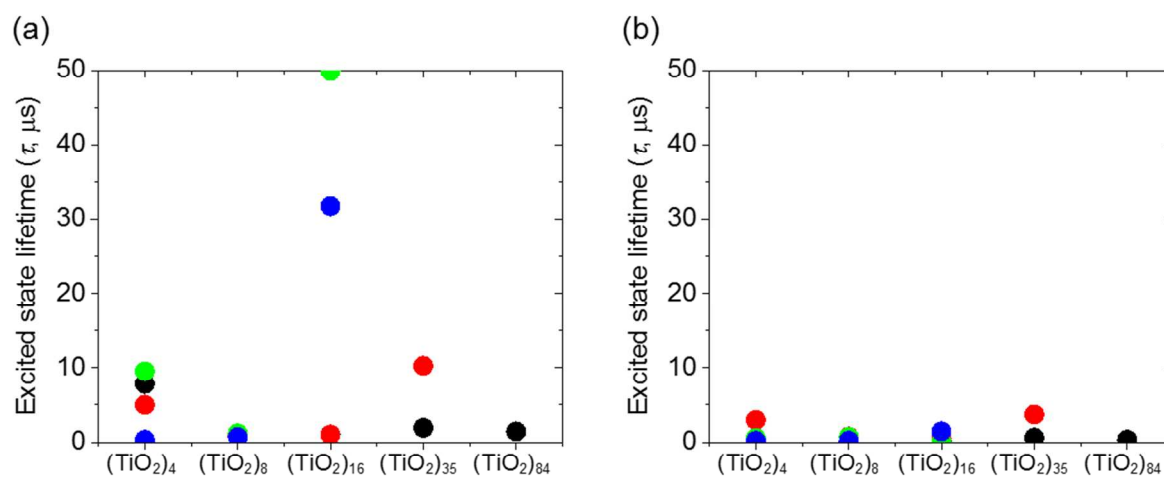


Figure S7. Excited state lifetime (τ) for the vertical S_1 exciton in (a) vacuum and (b) water calculated by B3LYP/6-31G(d) level.



6.1. Tables for excited state lifetime (τ) for vertical S_1 excitons in vacuum and water calculated by (CAM-)B3LYP/6-31G(d) level.

Table S12. Oscillator strength ($f_{(0 \rightarrow 1)v}$), ($S_0 \rightarrow S_1$)_v excitation energy, excited state lifetime ($\tau_{(1 \rightarrow 0)v}$) for the ($S_0 \rightarrow S_1$)_v excitation of the TiO₂ nanoparticles in vacuum calculated by CAM-B3LYP/6-31G(d) level.

	4unit				8unit				16unit				35unit				84unit	
	a (GM)	b	c	d ^a	a (GM) _a	b	c	d	a (GM)	b ^a	c	d	G09-Opt	Aims	Aims			
# of TiO2 units	4	4	4	4	8	8	8	8	16	16	16	16	35	35	84			
$f_{(0 \rightarrow 1)v}$	1×10^{-4}	7×10^{-4}	1×10^{-3}	3×10^{-3}	5×10^{-5}	3×10^{-4}	3×10^{-4}	2×10^{-3}	2×10^{-3}	4×10^{-3}	3×10^{-5}	4×10^{-4}	6×10^{-4}	1×10^{-3}	2×10^{-3}			
$(S_0 \rightarrow S_1)_v$ (eV)	4.411	4.037	3.823	4.232	4.777	4.789	4.347	4.720	4.740	4.902	4.648	4.239	4.519	3.885	4.169			
$\tau_{(1 \rightarrow 0)v}$ (μs)	12.5	2.1	1.5	0.5	20.5	3.0	4.4	0.5	0.4	0.2	41.3	3.0	1.9	1.2	0.8			

^a Excited state lifetime for the ($S_0 \rightarrow S_2$)_v excitation was reported as the oscillator strength ($f_{(0 \rightarrow 1)}$) for ($S_0 \rightarrow S_1$)_v excitation was so small ($< 1 \times 10^{-9}$) that probability for the generation of ($S_0 \rightarrow S_1$)_v exciton is negligible in general. Furthermore, as the ($S_0 \rightarrow S_1$)_v and ($S_0 \rightarrow S_2$)_v energies are almost degenerate (< 0.024 eV), ($S_0 \rightarrow S_2$)_v excitation has no energetic disadvantage over ($S_0 \rightarrow S_1$)_v excitation.

Table S13. Oscillator strength ($f_{(0 \rightarrow 1)v}$), ($S_0 \rightarrow S_1$)_v excitation energy, excited state lifetime ($\tau_{(1 \rightarrow 0)v}$) for the ($S_0 \rightarrow S_1$)_v excitation of the TiO₂ nanoparticles in water calculated by CAM-B3LYP/6-31G(d) level.

	4unit				8unit				16unit				35unit				84unit	
	a (GM)	b	c	d ^a	a (GM) _a	b	c	d	a (GM)	b	c ^a	d	G09-Opt	Aims	Aims			
# ofTiO2 units	4	4	4	4	8	8	8	8	16	16	16	16	35	35	84			
f _{(0→1)v}	4×10 ⁻³	1×10 ⁻³	2×10 ⁻³	5×10 ⁻³	2×10 ⁻⁴	2×10 ⁻³	2×10 ⁻³	1×10 ⁻³	1×10 ⁻²	2×10 ⁻²	4×10 ⁻²	9×10 ⁻⁴	2×10 ⁻²	2×10 ⁻³	1×10 ⁻²			
(S ₀ →S ₁) _v	4.716	4.350	4.825	5.090	4.878	4.883	4.613	4.870	4.771	4.954	4.886	4.331	4.544	4.209	4.192			
τ _{(1→0)v} (us)	0.2	0.9	0.4	0.1	4.0	0.4	0.5	0.5	0.1	0.04	0.02	1.0	0.05	0.5	0.1			

^a Excited state lifetime for the ($S_0 \rightarrow S_2$)_v excitation was reported as the oscillator strength ($f_{(0 \rightarrow 1)}$) for ($S_0 \rightarrow S_1$)_v excitation was so small ($< 1 \times 10^{-9}$) that probability for the generation of ($S_0 \rightarrow S_1$)_v exciton is negligible in general. Furthermore, as the ($S_0 \rightarrow S_1$)_v and ($S_0 \rightarrow S_2$)_v energies are almost degenerate (< 0.044 eV), ($S_0 \rightarrow S_2$)_v excitation has no energetic disadvantage over ($S_0 \rightarrow S_1$)_v excitation.

Table S14. Oscillator strength ($f_{(0 \rightarrow 1)v}$), ($S_0 \rightarrow S_1$)_v excitation energy, excited state lifetime ($\tau_{(1 \rightarrow 0)v}$) for the ($S_0 \rightarrow S_1$)_v excitation of the TiO₂ nanoparticles in vacuum calculated by B3LYP/6-31G(d) level.

	4unit				8unit				16unit				35unit			84unit
	a (GM) ^a	b	c	d ^a	a (GM)	b	c	d	a (GM)	b	c	d	G09-Opt	Aims	Aims	
# of TiO ₂ units	4	4	4	4	8	8	8	8	16	16	16	16	35	35	84	
$f_{(0 \rightarrow 1)v}$	2×10^{-4}	4×10^{-4}	4×10^{-4}	5×10^{-3}	1×10^{-3}	2×10^{-3}	1×10^{-3}	2×10^{-3}	2×10^{-3}	1×10^{-3}	3×10^{-5}	1×10^{-4}	9×10^{-4}	2×10^{-4}	1×10^{-3}	
($S_0 \rightarrow S_1$) _v	3.938	3.558	2.412	3.816	4.112	3.850	3.867	3.787	3.610	4.077	4.132	2.366	3.669	3.364	3.397	
$\tau_{(1 \rightarrow 0)v}$ (μs)	7.8	5.0	9.5	0.3	1.1	0.9	1.2	0.7	1.0	1.0	49.9	31.8	1.9	10.3	1.4	

^a Excited state lifetime for the ($S_0 \rightarrow S_2$)_v excitation was reported as the oscillator strength ($f_{(0 \rightarrow 1)}$) for ($S_0 \rightarrow S_1$)_v excitation was so small ($< 1 \times 10^{-9}$) that probability for the generation of ($S_0 \rightarrow S_1$)_v exciton is negligible in general. Furthermore, as the ($S_0 \rightarrow S_1$)_v and ($S_0 \rightarrow S_2$)_v energies are almost degenerate (< 0.015 eV), ($S_0 \rightarrow S_2$)_v excitation has no energetic disadvantage over ($S_0 \rightarrow S_1$)_v excitation.

Table S15. Oscillator strength ($f_{(0 \rightarrow 1)v}$), ($S_0 \rightarrow S_1$)_v excitation energy, excited state lifetime ($\tau_{(1 \rightarrow 0)v}$) for the ($S_0 \rightarrow S_1$)_v excitation of the TiO₂ nanoparticles in water calculated by B3LYP/6-31G(d) level.

	4unit				8unit				16unit				35unit			84unit
	a (GM)	b	c	d ^a	a (GM) ^a	b	c	d	a (GM)	b	c ^a	d	G09-Opt	Aims	Aims	
# of TiO ₂ units	4	4	4	4	8	8	8	8	16	16	16	16	35	35	84	
$f_{(0 \rightarrow 1)v}$	5×10^{-3}	4×10^{-4}	2×10^{-3}	4×10^{-3}	2×10^{-2}	1×10^{-3}	1×10^{-3}	5×10^{-3}	5×10^{-3}	2×10^{-3}	2×10^{-2}	9×10^{-4}	2×10^{-3}	4×10^{-4}	4×10^{-3}	
($S_0 \rightarrow S_1$) _v (eV)	4.259	3.883	4.306	4.665	4.342	4.338	4.117	4.310	4.050	4.325	4.242	3.607	3.694	3.431	3.434	
$\tau_{(1 \rightarrow 0)v}$ (μs)	0.2	3.0	0.6	0.2	0.04	0.8	0.7	0.2	0.2	0.5	0.05	1.4	0.6	3.7	0.3	

^a Excited state lifetime for the ($S_0 \rightarrow S_2$)_v excitation was reported as the oscillator strength ($f_{(0 \rightarrow 1)}$) for ($S_0 \rightarrow S_1$)_v excitation was so small ($< 1 \times 10^{-9}$) that probability for the generation of ($S_0 \rightarrow S_1$)_v exciton is negligible in general. Furthermore, as the ($S_0 \rightarrow S_1$)_v and ($S_0 \rightarrow S_2$)_v energies are almost degenerate (< 0.076 eV), ($S_0 \rightarrow S_2$)_v excitation has no energetic disadvantage over ($S_0 \rightarrow S_1$)_v excitation.

6.2. Tables for excited state lifetime (τ) for relaxed S_1 excitons in vacuum and water calculated by CAM-B3LYP/6-31G(d) level.

Table S16. Oscillator strength ($f_{(0 \rightarrow 1)ad}$), ($S_0 \rightarrow S_1$)_{ad} excitation energy, excited state lifetime ($\tau_{(1 \rightarrow 0),ad}$) for the ($S_0 \rightarrow S_1$)_{ad} excitation of the TiO₂ nanoparticles in vacuum calculated by CAM-B3LYP/6-31G(d) level.

	4unit				8unit				16unit				35unit		84unit
	a (GM)	b	c	d	a (GM)	b ^a	c	d	a (GM)	b	c	d ^a	G09-Opt	Aims	Aims
# of TiO ₂ units	4	4	4	4	8	8	8	8	16	16	16	16	35	35	84
$f_{(0 \rightarrow 1)ad}$	2×10^{-4}	6×10^{-4}	5×10^{-3}	1×10^{-4}	1×10^{-4}	2×10^{-3}	9×10^{-4}	1×10^{-4}	2×10^{-4}	9×10^{-4}	1×10^{-3}	3×10^{-3}			
($S_0 \rightarrow S_1$) _{ad} (eV)	2.571	2.443	2.239	2.931	3.328	3.923	2.496	2.715	2.483	2.780	3.091	2.799			
$\tau_{(1 \rightarrow 0)ad}$ (μ s)	17.6	6.5	1.0	27.1	21.0	0.840	4.2	31.6	18.9	3.3	2.4	1.1			

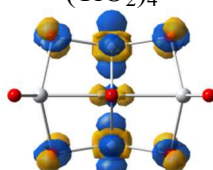
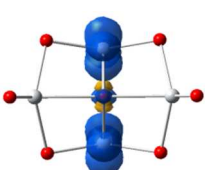
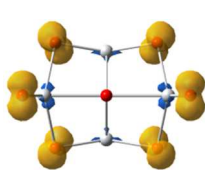
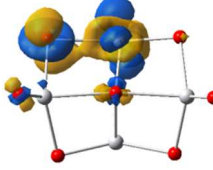
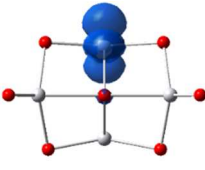
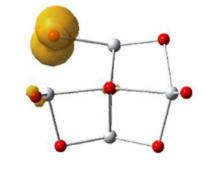
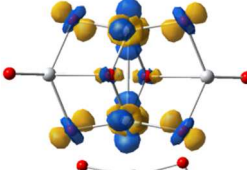
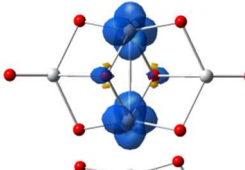
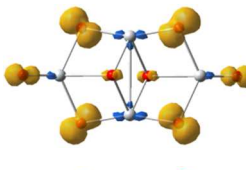
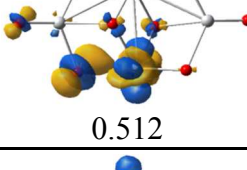
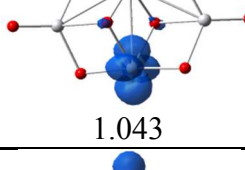
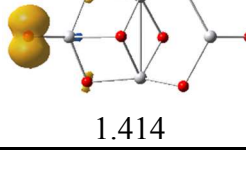
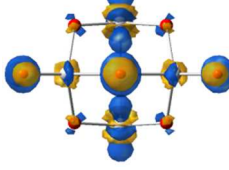
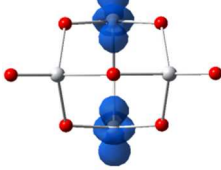
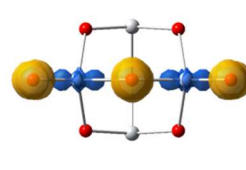
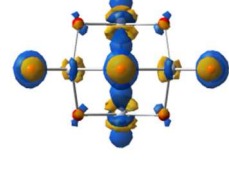
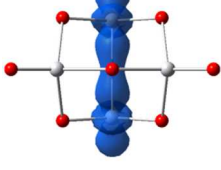
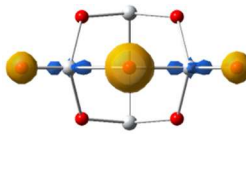
^a Excited state lifetime for the ($S_0 \rightarrow S_2$)_{ad} excitation was reported as the oscillator strength ($f_{(0 \rightarrow 1)ad}$) for ($S_0 \rightarrow S_1$)_{ad} excitation was so small ($< 1 \times 10^{-17}$) that radiative decay proceed through ($S_2 \rightarrow S_0$)_{ad} exciton pathway. Energy difference between ($S_0 \rightarrow S_1$)_{ad} and ($S_0 \rightarrow S_2$)_{ad} energies are smaller than 0.655 eV.

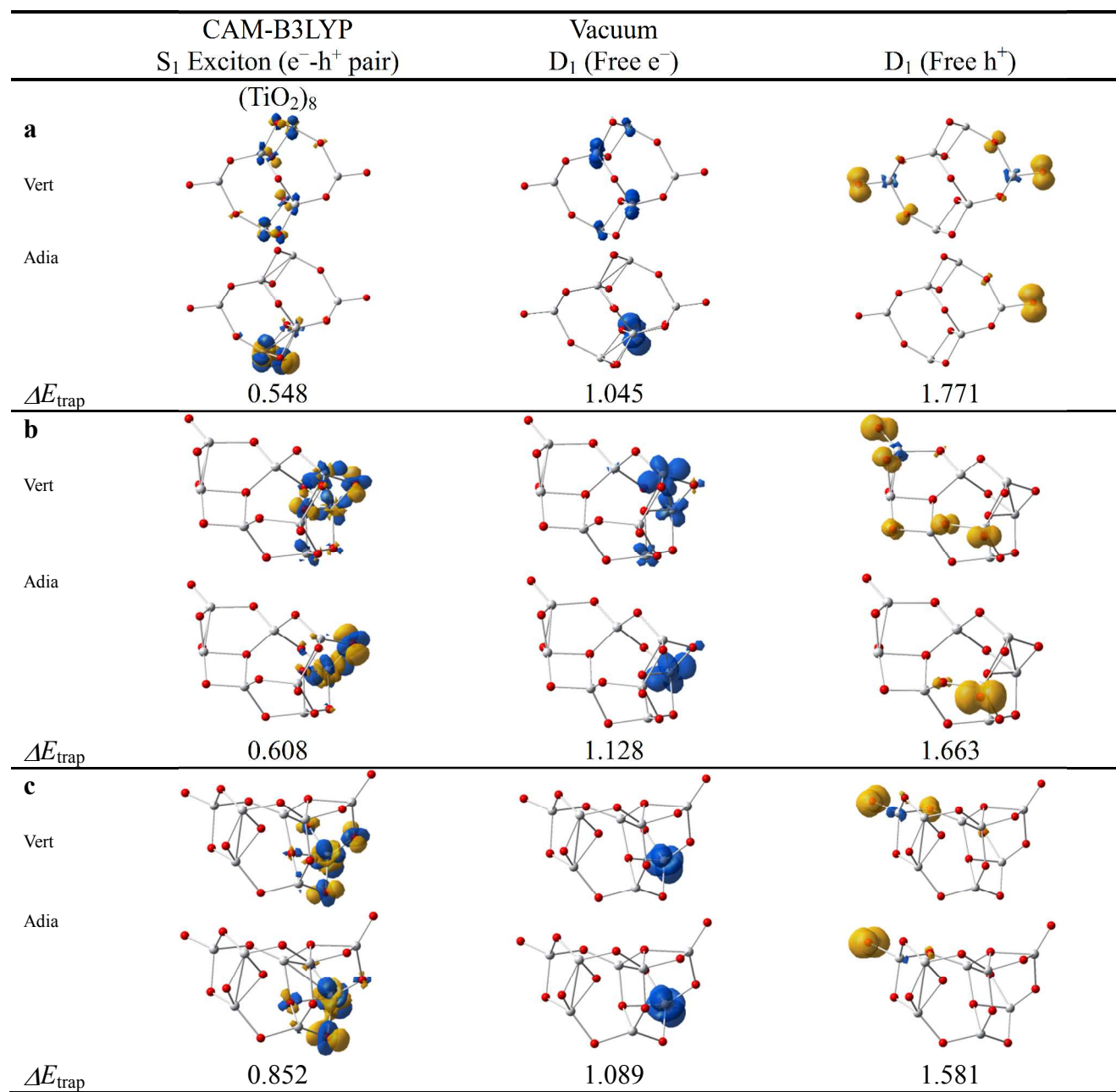
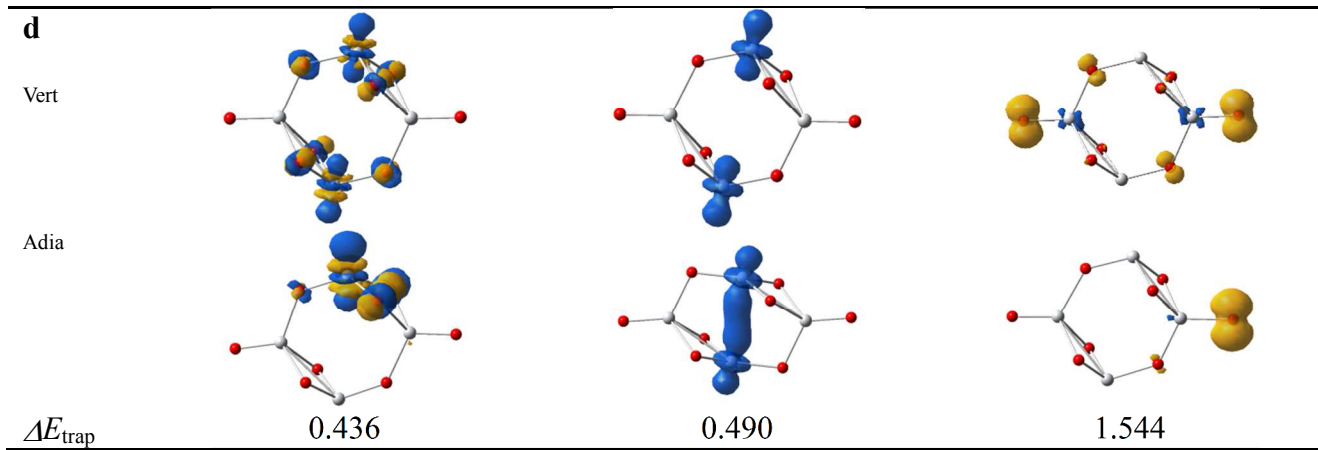
Table S17. Oscillator strength ($f_{(0 \rightarrow 1)ad}$), ($S_0 \rightarrow S_1$)_{ad} excitation energy, excited state lifetime ($\tau_{(1 \rightarrow 0),ad}$) of the TiO₂ nanoparticles in water calculated by CAM-B3LYP/6-31G(d) level.

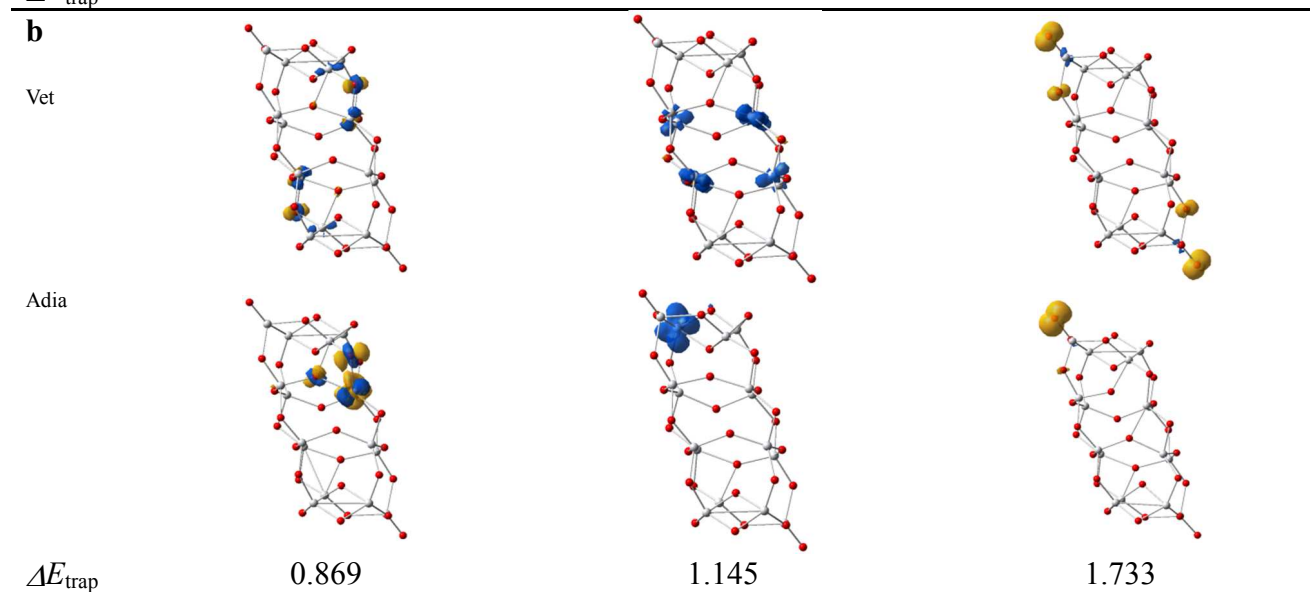
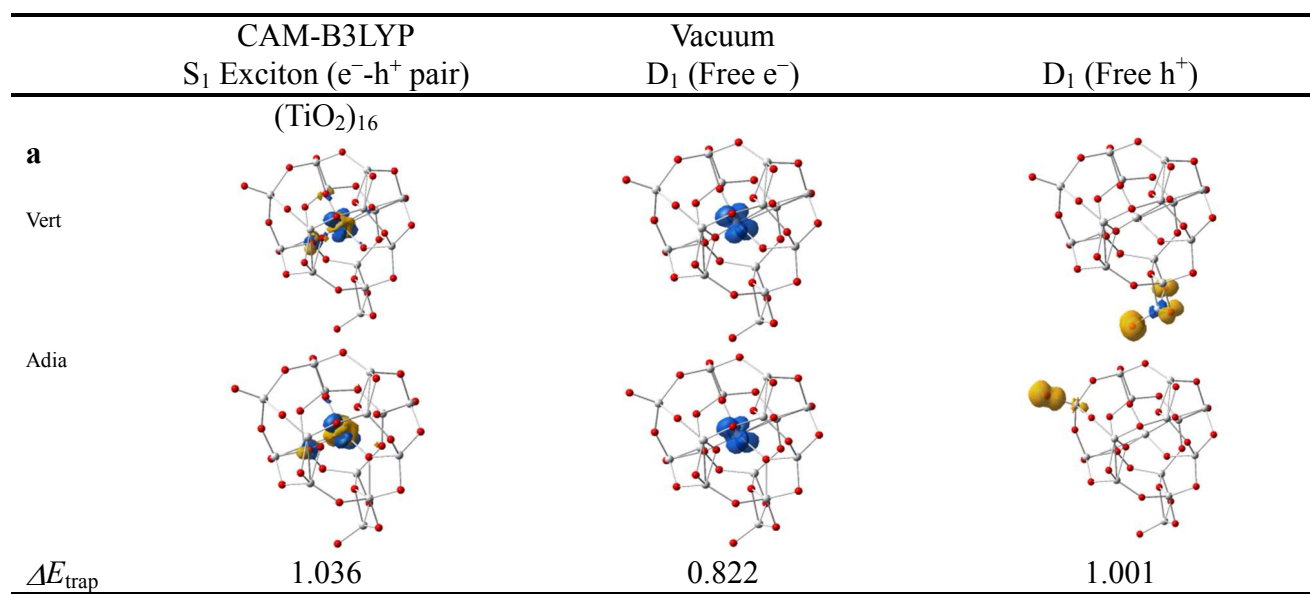
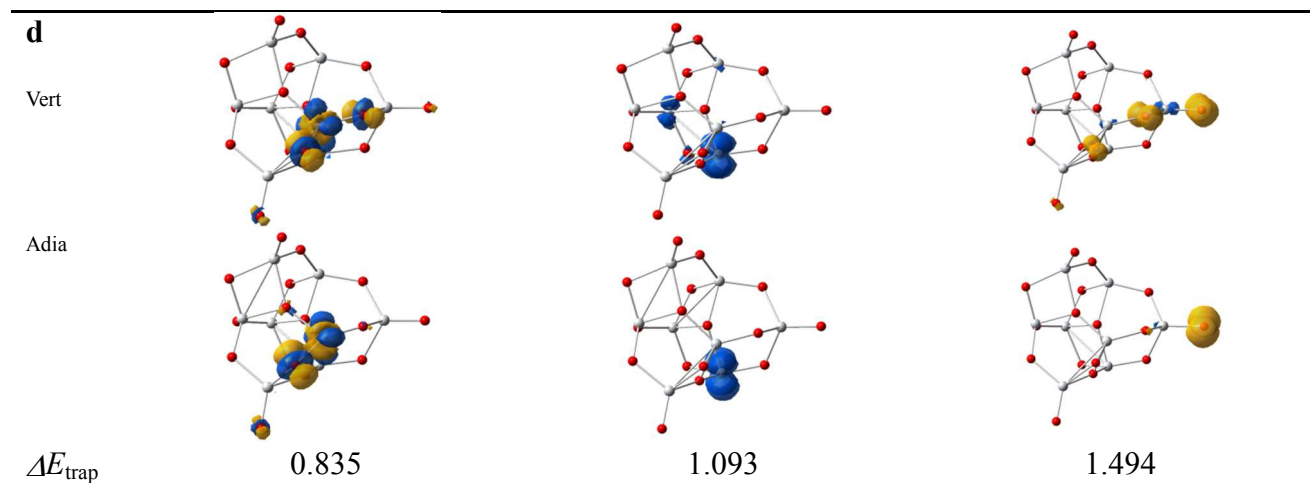
	4unit				8unit				16unit				35unit		84unit
	a (GM)	b	c	d	a (GM)	b	c	d	a (GM)	b	c	d	G09-Opt	Aims	Aims
# of TiO ₂ units	4	4	4	4	8	8	8	8	16	16	16	16	35	35	84
$f_{(0 \rightarrow 1)ad}$	2×10^{-4}	1×10^{-3}	1×10^{-2}	1×10^{-4}	4×10^{-4}	2×10^{-4}	2×10^{-3}	3×10^{-4}	7×10^{-4}	3×10^{-3}	3×10^{-3}	1×10^{-4}			
($S_0 \rightarrow S_1$) _{ad} (eV)	3.199	3.074	3.905	3.728	3.650	3.655	3.073	3.271	2.664	3.061	3.308	2.433			
$\tau_{(1 \rightarrow 0)ad}$ (μ s)	8.5	1.7	0.1	12.6	3.3	6.5	0.8	5.4	3.5	0.6	0.6	29.5			

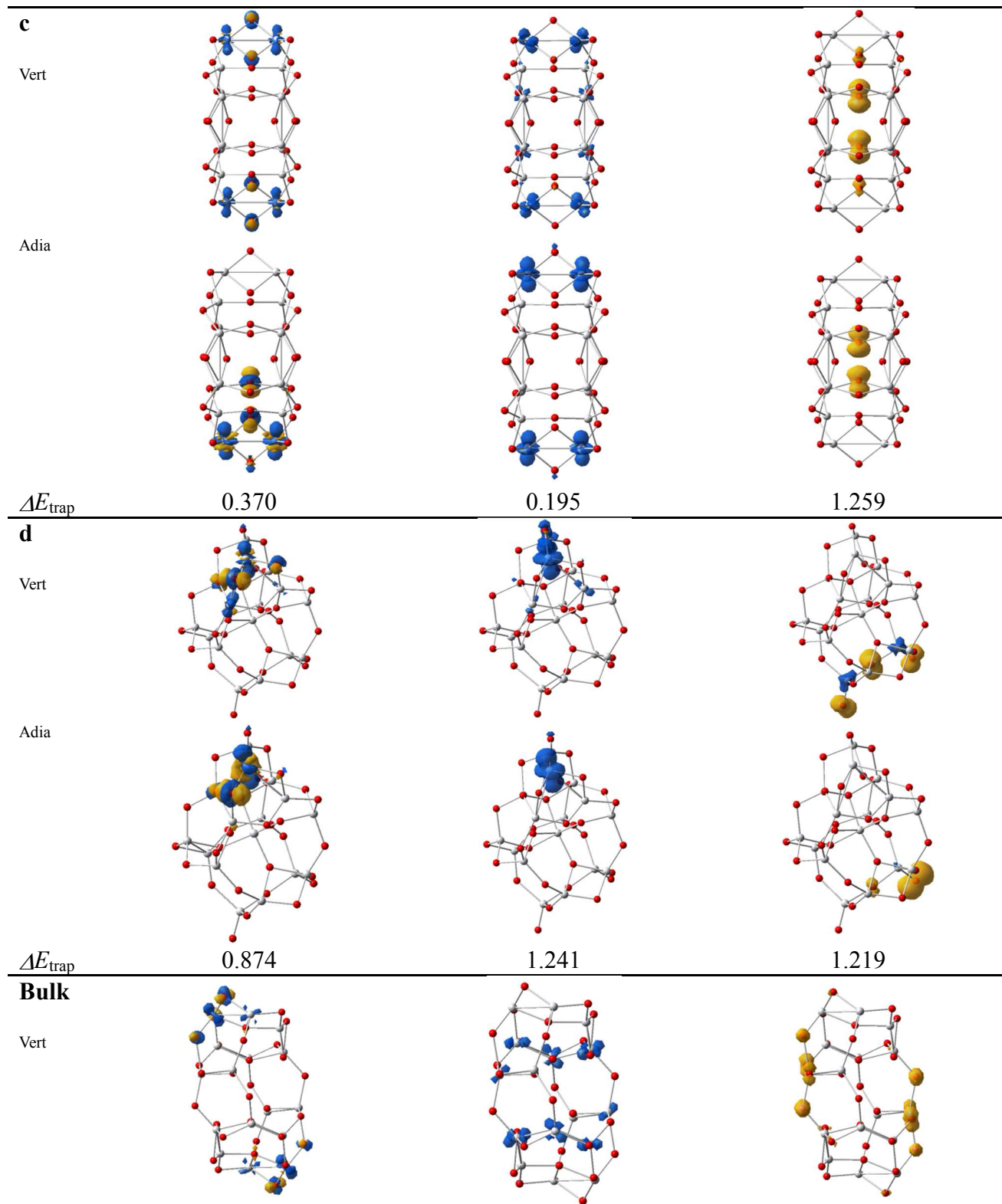
7. Calculated electron and hole distributions in S_1 exciton and free charge carrier in vacuum and water obtained by (CAM-)B3LYP/6-31G(d) level.

Figure S8. Calculated S_1 exciton pair (left panel), free electron (middle panel) and free hole (right panel) distributions (isovalue = $0.01 \text{ e}^- \text{au}^{-3}$) created by vertical and adiabatic transitions in vacuum at CAM-B3LYP/6-31G(d) level. Self-trapping energies ($\Delta E_{\text{trap}} = E_{\text{vert}} - E_{\text{adia}}$) are also given. Blue and yellow lobes represent excited electron and hole densities, respectively.

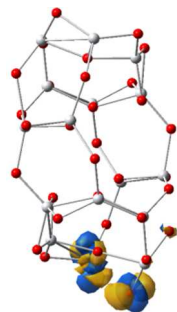
	CAM-B3LYP S_1 Exciton ($\text{e}^- \text{-h}^+$ pair)	Vacuum D_1 (Free e^-)	D_1 (Free h^+)
a			
	(TiO_2) ₄		
Vert			
Adia			
ΔE_{trap}	0.721	1.148	0.911
b			
Vert			
Adia			
ΔE_{trap}	0.512	1.043	1.414
c			
Vert			
Adia			
ΔE_{trap}	0.793	0.605	0.258



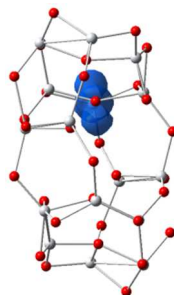




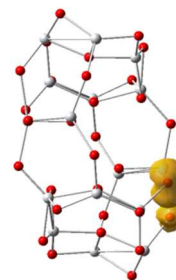
Adia



0.539



1.354



1.438

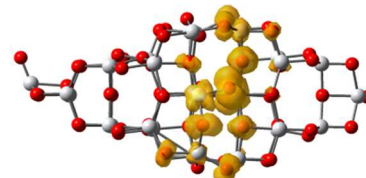
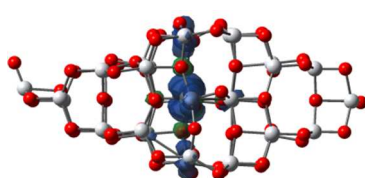
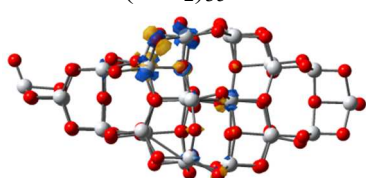
 ΔE_{trap}

CAM-B3LYP
S₁ Exciton (e⁻-h⁺ pair)
(TiO₂)₃₅^a

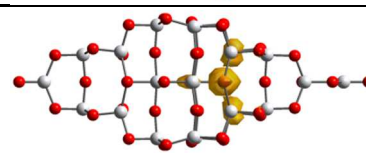
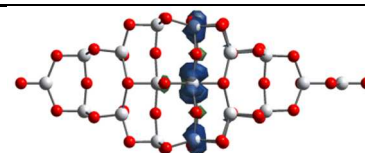
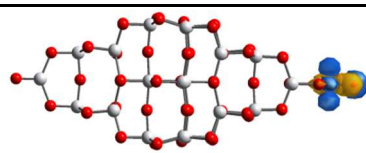
Vacuum
D₁ (Free e⁻)

D₁ (Free h⁺)**a**

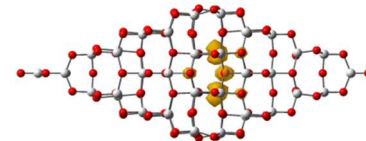
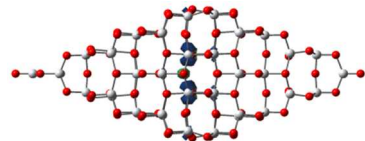
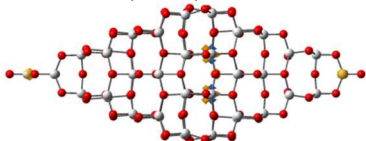
Vert

**b**

Vert

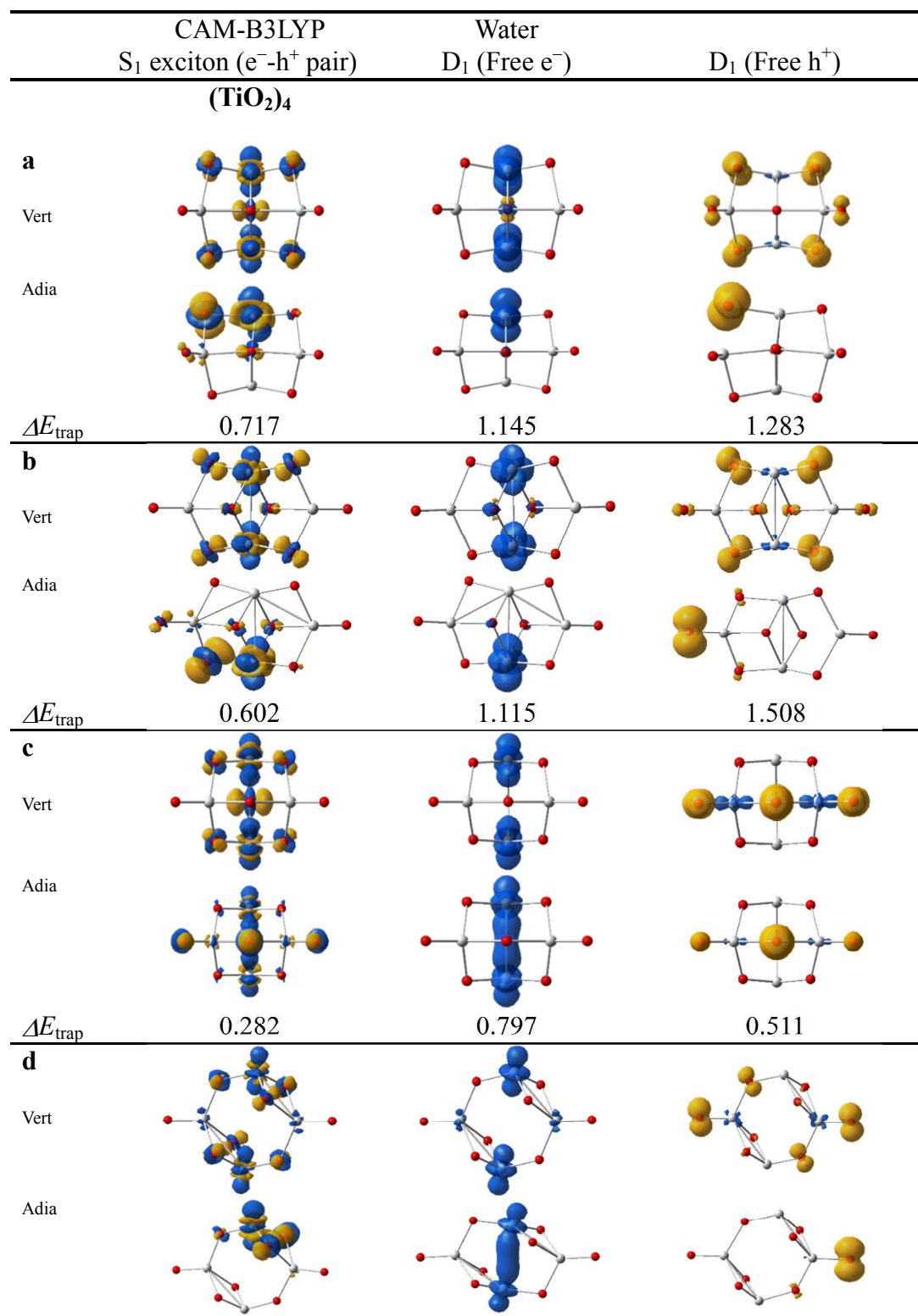
(TiO₂)₈₄^a**a**

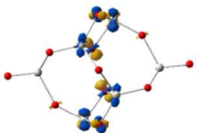
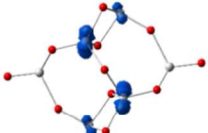
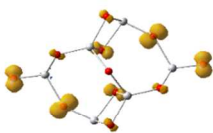
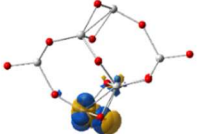
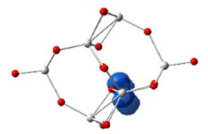
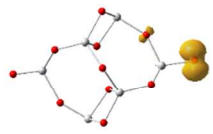
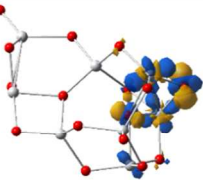
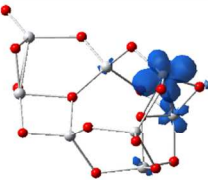
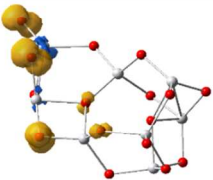
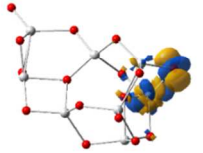
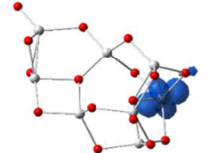
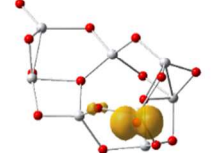
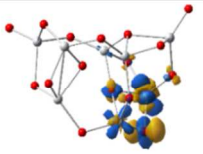
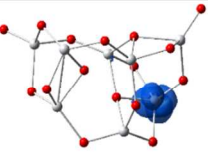
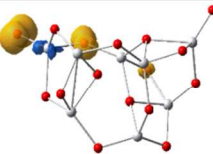
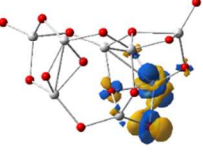
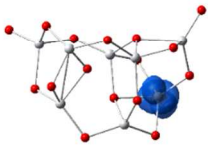
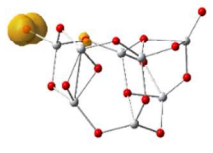
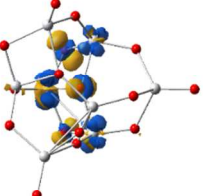
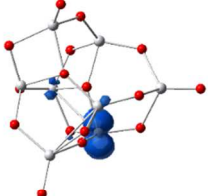
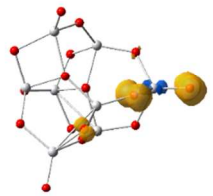
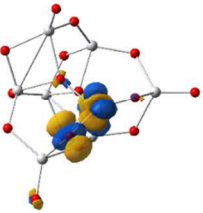
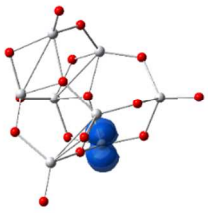
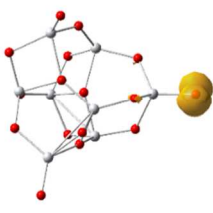
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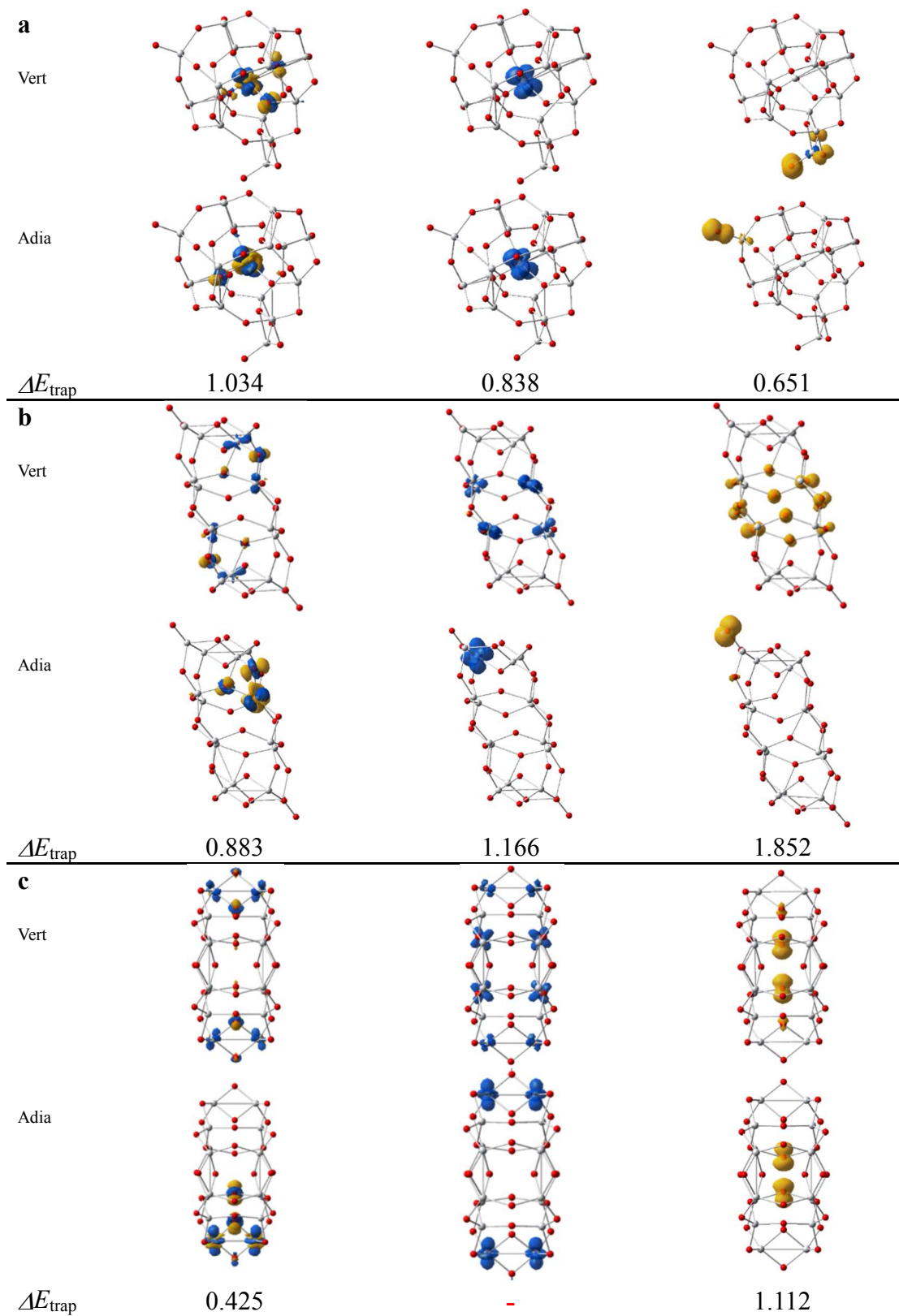


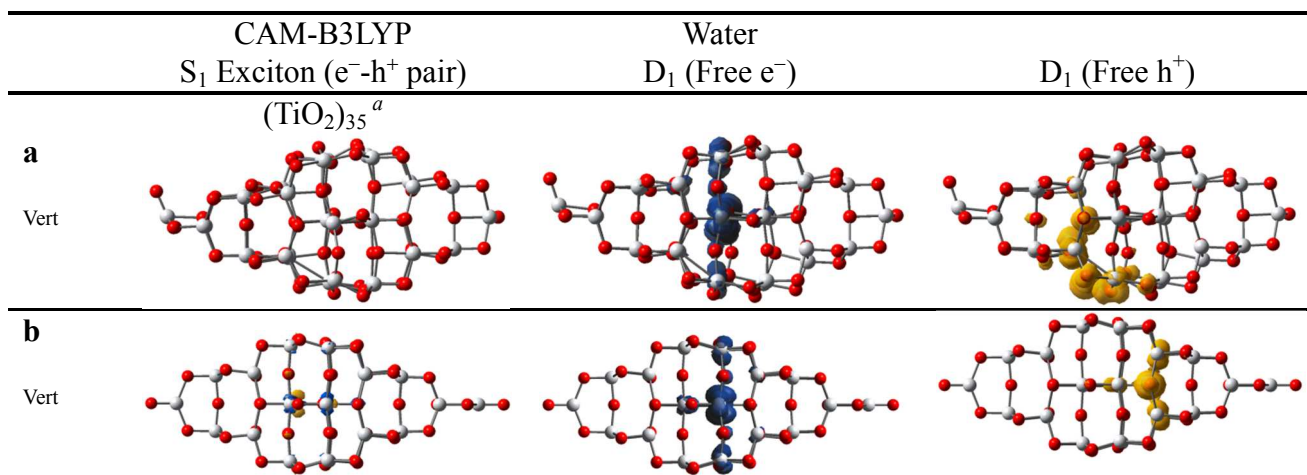
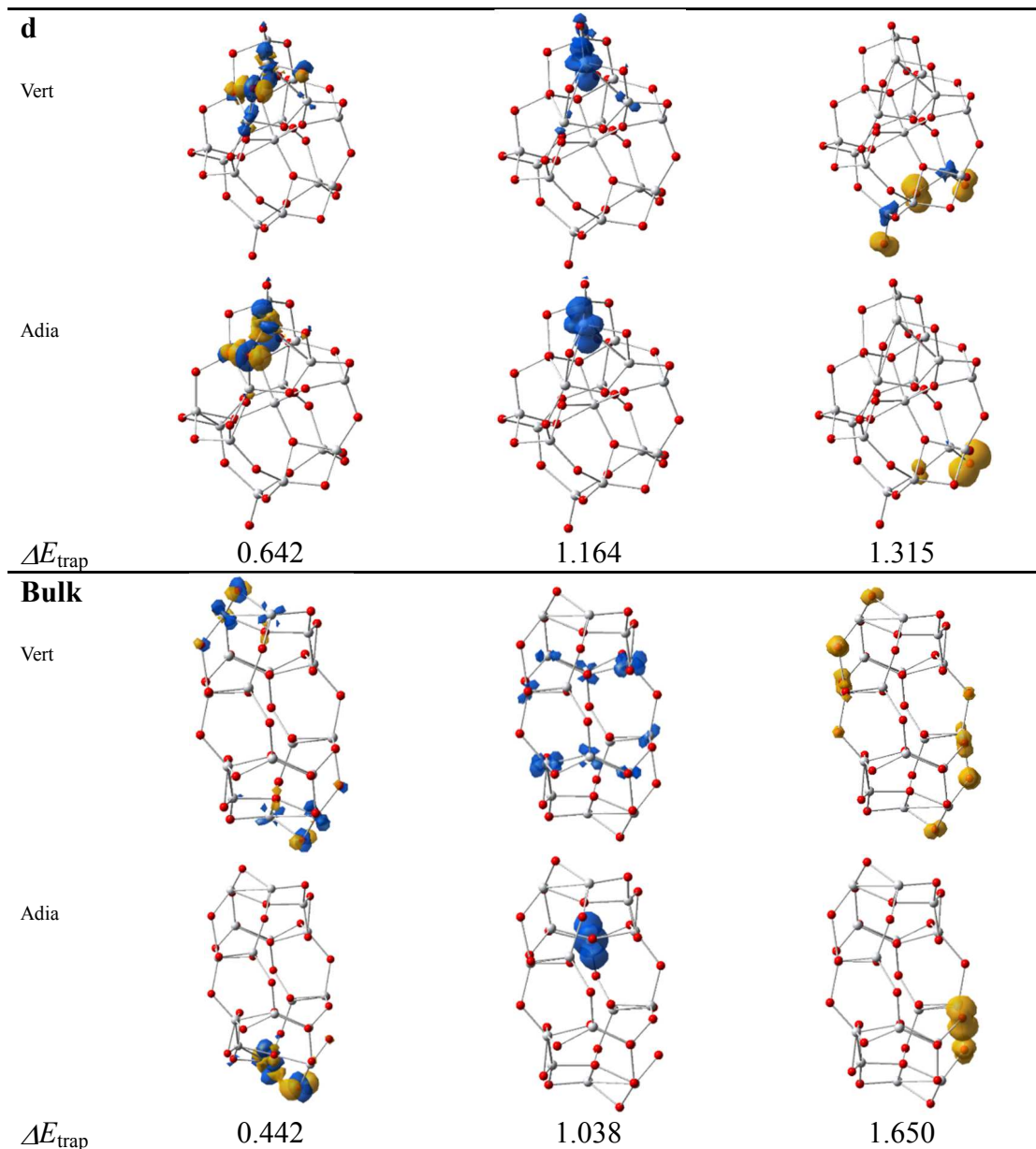
^a Calculated S₁ exciton pair, and free electron and hole distributions in (TiO₂)_{35a,35b,84} are drawn for isovalue of 0.004 and 0.001 e⁻·au⁻³, respectively.

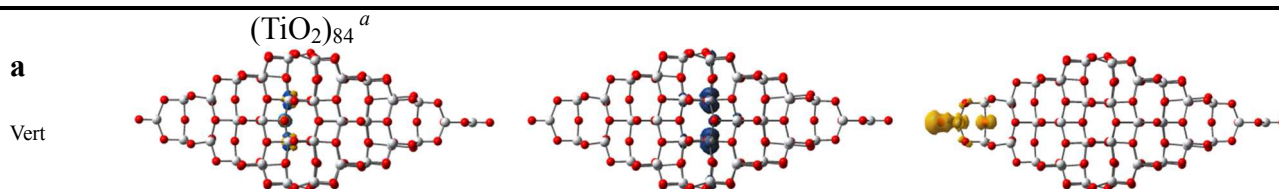
Figure S9. Calculated S_1 exciton pair (left panel), free electron (middle panel) and free hole (right panel) distributions (isovalue = $0.01 \text{ e}^- \text{au}^{-3}$) created by vertical and adiabatic transitions in water at CAM-B3LYP/6-31G(d) level. Self-trapping energies ($\Delta E_{\text{trap}} = E_{\text{vert}} - E_{\text{adia}}$) are also given. Blue and yellow lobes represent excited electron and hole densities, respectively.



ΔE_{trap}	0.553	0.170	1.838
	CAM-B3LYP	Water	
	S_1 Exciton (e^- - h^+ pair)	D_1 (Free e^-)	D_1 (Free h^+)
(TiO₂)₈			
a			
Vert			
Adia			
ΔE_{trap}	0.416	1.143	1.924
b			
Vert			
Adia			
ΔE_{trap}	0.517	1.075	1.814
c			
Vert			
Adia			
ΔE_{trap}	0.594	1.082	1.751
d			
Vert			
Adia			
ΔE_{trap}	0.856	1.184	1.612
	CAM-B3LYP	Water	
	S_1 Exciton (e^- - h^+ pair)	D_1 (Free e^-)	D_1 (Free h^+)
(TiO₂)₁₆			







^a Calculated S₁ exciton pair, and free electron and hole distributions in (TiO₂)_{35a,35b,84} are drawn for isovalue of 0.004 and 0.001 e⁻au⁻³, respectively.

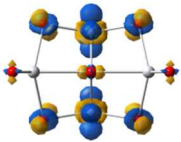
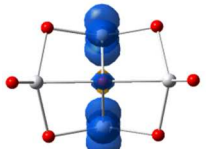
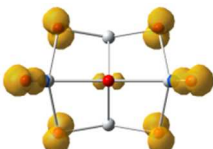
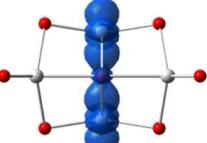
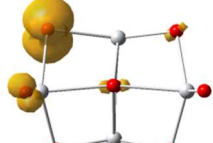
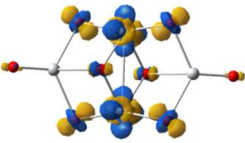
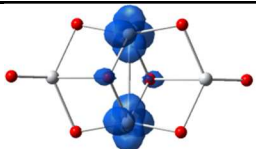
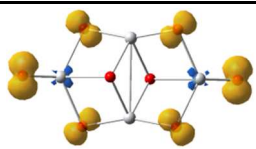
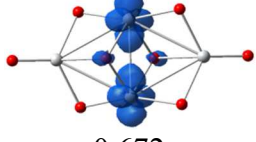
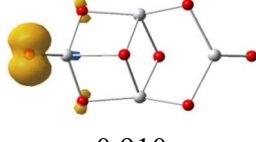
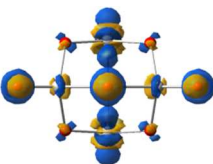
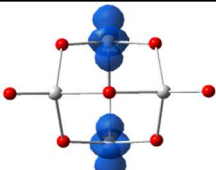
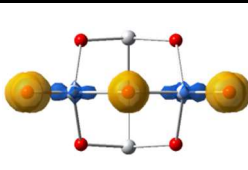
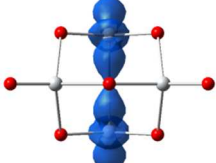
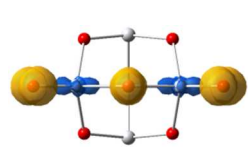
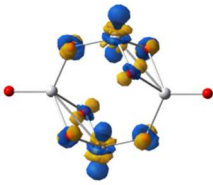
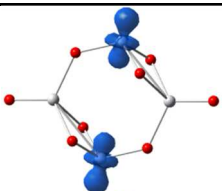
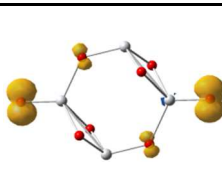
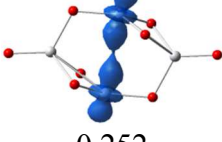
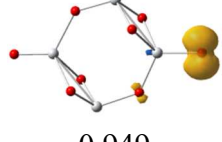
Electron-hole Distributions. The S₁ exciton and the free charge carriers are species to facilitate photocatalytic reaction. However, electron-hole recombination is a kinetic factor and is a limiting condition for photocatalytic efficiency. After electron-hole recombination it becomes impossible to promote the photocatalytic reactions. Therefore, suppression of the electron-hole recombination through the spatial separation of excited electron and hole components are of particular importance. In this purpose, spatial distribution of S₁ exciton state was obtained by the difference density between S₁ and corresponding S₀ states, and the free electron/hole distributions were drawn from electron spin density plots of free electron/hole states. However, one should note that the limitations of the CPCM model imply that the results may include unavoidable artifacts such as localization of free electron/hole to the structural defects such as under-coordinated titanium/oxygen which may be hydrated when immersed in water.

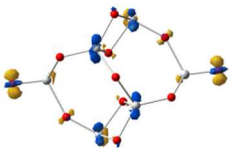
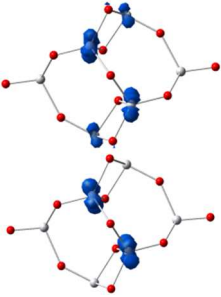
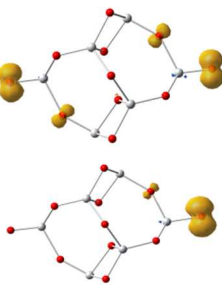
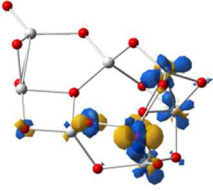
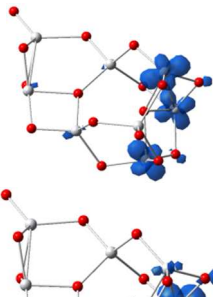
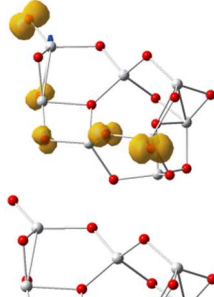
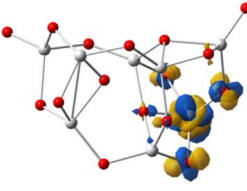
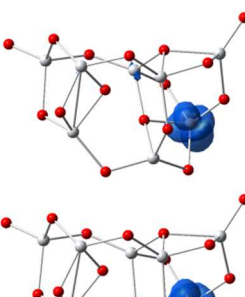
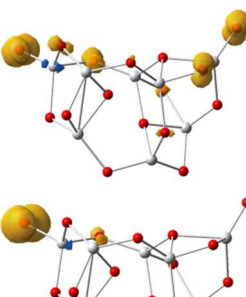
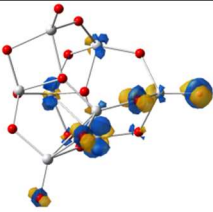
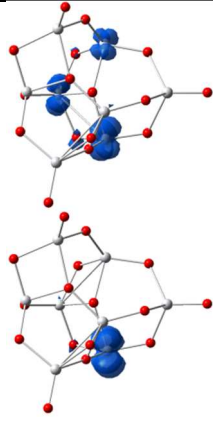
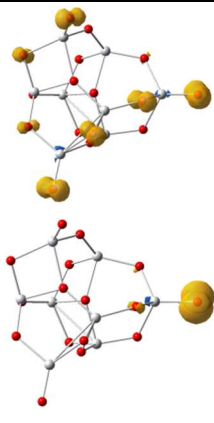
Figures S8-S9 and S10-S11 show the spatial distributions of excited electron (blue) and hole (yellow) in S₁ exciton, free electron, and free hole states obtained by CAM-B3LYP and B3LYP functionals, respectively. We will mainly discuss the electron/hole behaviors presented in Figure S8 and S9 (CAM-B3LYP), since the similar discussions are also applicable to S10 and S11 (B3LYP), respectively. First of all, excess electron and hole distributions in vacuum and water shows qualitatively similar patterns, despite the electron reorganization occurs upon CPCM water solvation (as mentioned in Supporting Information Section 4). Noticeable localization of excited electron to (mostly three-coordinated) Ti sites and hole to (mostly mono-coordinated) O sites were observed in most of the TiO₂ NPs. Upon geometric

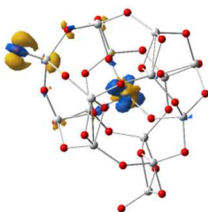
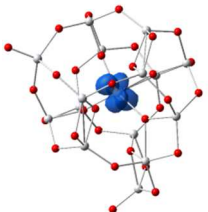
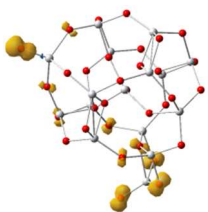
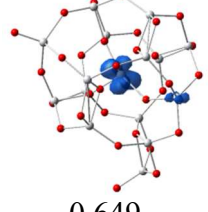
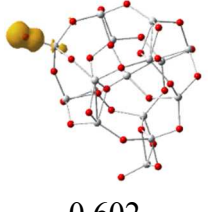
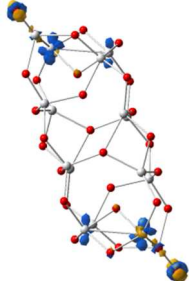
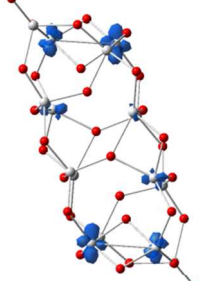
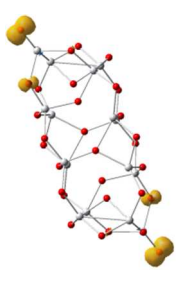
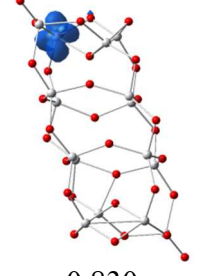
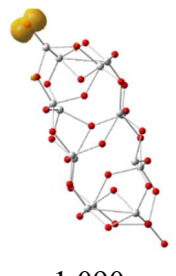
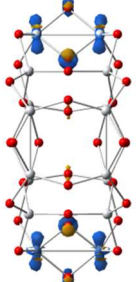
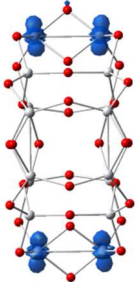
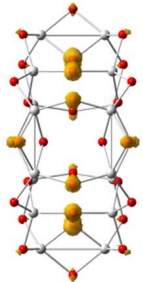
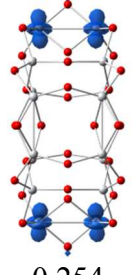
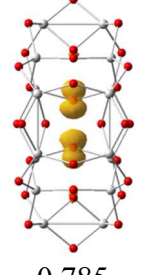
relaxation, vertically excited electron and hole species further localized into a fewer atoms. Then, the defect sites possessing extra electron/hole will play as a reaction center for HER/OER half-reactions. In other words, electron and hole species are more efficiently separated in free charge carrier states and electron-hole pair in S_1 exciton have close proximity, which may ascribe to electrostatic stabilization in a close electron-hole distance. Generally, the electron-hole become more delocalized through the larger space in bigger nanoparticles (TiO_2)_{35,84}, which led to weak electron-hole interactions in S_1 exciton (small exciton binding energy ΔE_{ex}). We note that the electron-hole distributions of TiO_2 nanoparticles in CPCM water model (Figure S9 and S11) may be changed when considering explicit water solvent and hydration of the under-coordinated defect species.

Self-trapping energy ($\Delta E_{\text{trap}} = E_{\text{vert}} - E_{\text{adia}}$) is a measure of stabilization of the total energy upon electron/hole localization in S_1 exciton or free charge carriers, from which we can extract the thermodynamic preference for the localized states. For S_1 exciton, ΔE_{trap} corresponds to reorganization energy in the S_1 excited state. The carrier localization was the most pronounced in free hole states as indicated by large positive ΔE_{trap} over 1 eV in the most of the NPs. The ΔE_{trap} of S_1 exciton states were often found to be the smallest except for a few cases. However, it is difficult to develop a quantitative relationship between ΔE_{trap} and reorganization of electron/hole distribution upon relaxation. Adiabatic free charge carriers become more stable than adiabatic S_1 exciton when the sum of the ΔE_{trap} of free electron and hole overwhelms the sum of ΔE_{trap} and ΔE_{ex} of S_1 exciton (as mentioned in the discussions regarding Figure 5b right panel).

Figure S10. Calculated S_1 exciton pair (left panel), free electron (middle panel) and free hole (right panel) distributions (isovalue = $0.01 \text{ e}^- \text{au}^{-3}$) created by vertical and adiabatic transitions in vacuum at B3LYP/6-31G(d) level. Self-trapping energies ($\Delta E_{\text{trap}} = E_{\text{vert}} - E_{\text{adia}}$) are also given. Blue and yellow lobes represent excited electron and hole densities, respectively.

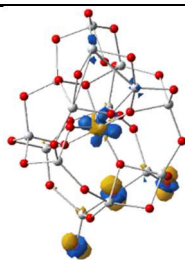
	B3LYP S_1 Exciton ($\text{e}^- \text{-h}^+$ pair) (TiO_2) ₄	Vacuum D_1 (Free e^-)	D_1 (Free h^+)
a			
Vert			
Adia			
ΔE_{trap}		0.823	0.371
b			
Vert			
Adia			
ΔE_{trap}		0.672	0.910
c			
Vert			
Adia			
ΔE_{trap}		0.465	0.213
d			
Vert			
Adia			
ΔE_{trap}		0.252	0.949

	B3LYP S ₁ Exciton (e ⁻ -h ⁺ pair) (TiO ₂) ₈	Vacuum D ₁ (Free e ⁻)	D ₁ (Free h ⁺)
a			
Vert			
Adia			
ΔE_{trap}		0.305	1.107
b			
Vert			
Adia			
ΔE_{trap}		0.717	0.937
c			
Vert			
Adia			
ΔE_{trap}		0.953	1.145
d			
Vert			
Adia			
ΔE_{trap}		0.731	0.940

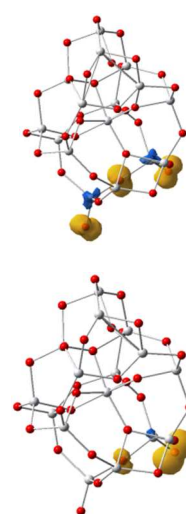
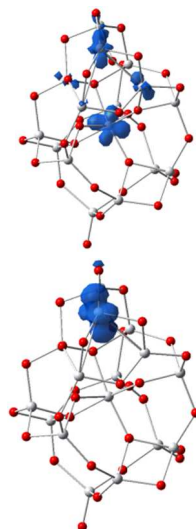
	B3LYP S ₁ Exciton (e ⁻ -h ⁺ pair) (TiO ₂) ₁₆	Vacuum D ₁ (Free e ⁻)	D ₁ (Free h ⁺)
a			
Vert			
Adia			
ΔE_{trap}		0.649	0.602
b			
Vert			
Adia			
ΔE_{trap}		0.830	1.090
c			
Vert			
Adia			
ΔE_{trap}		0.254	0.785

d

Vert



Adia

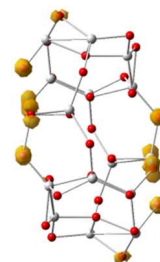
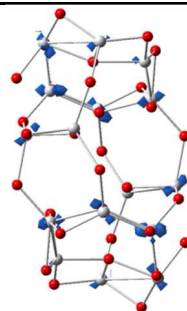
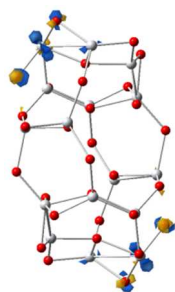
 ΔE_{trap}

0.767

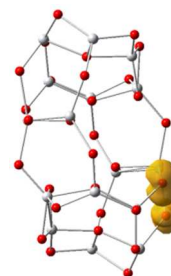
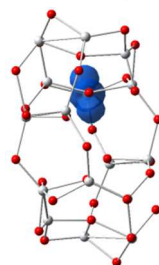
0.868

Bulk

Vert

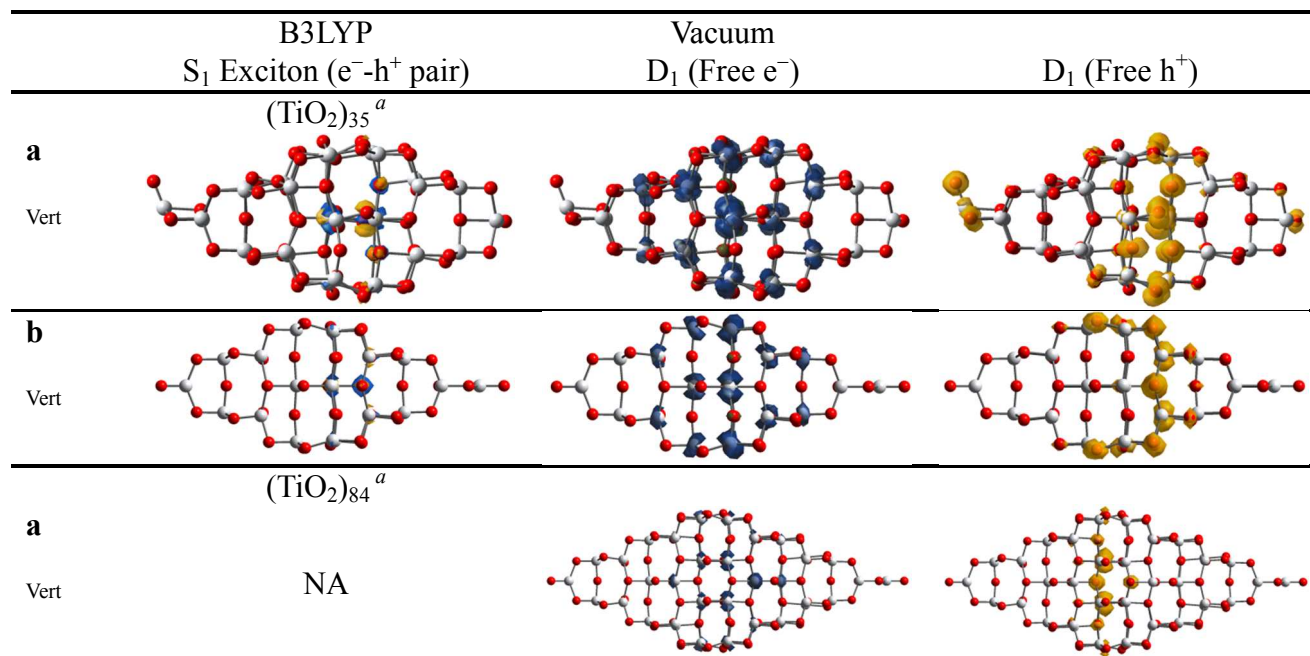


Adia

 ΔE_{trap}

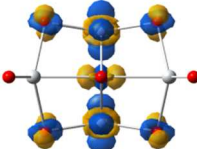
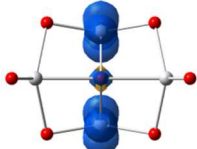
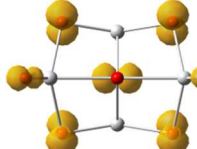
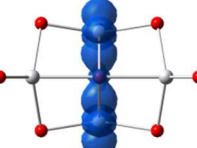
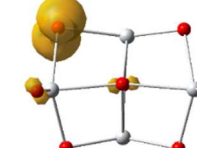
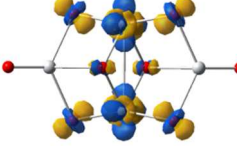
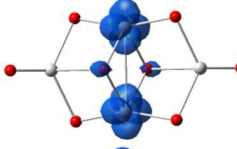
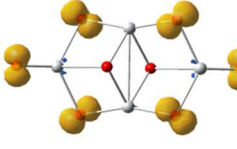
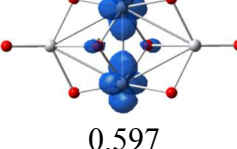
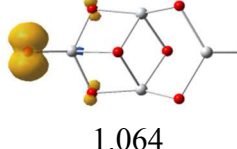
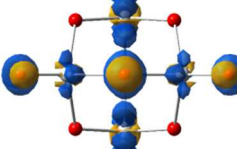
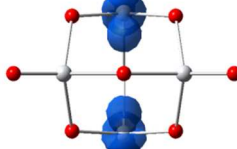
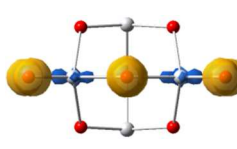
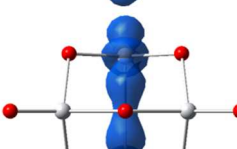
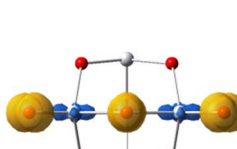
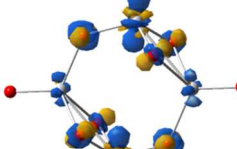
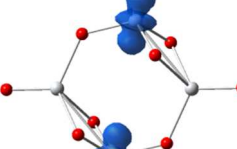
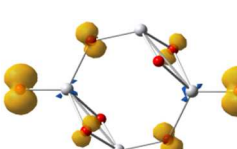
0.587

0.686

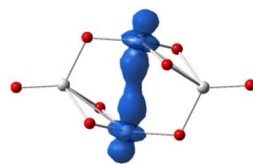


^a Calculated S₁ exciton pair, and free electron and hole distributions in (TiO₂)_{35a,35b,84} are drawn for isovalue of 0.004 and 0.001 e⁻·au⁻³, respectively.

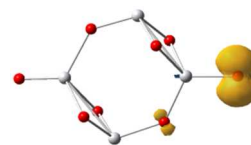
Figure S11. Calculated S_1 exciton pair (left panel), free electron (middle panel) and free hole (right panel) distributions (isovalue = $0.01 \text{ e}^- \text{au}^{-3}$) created by vertical and adiabatic transitions in water at B3LYP/6-31G(d) level. Self-trapping energies ($\Delta E_{\text{trap}} = E_{\text{vert}} - E_{\text{adia}}$) are also given. Blue and yellow lobes represent excited electron and hole densities, respectively.

	B3LYP S_1 Exciton ($\text{e}^- \text{-h}^+$ pair)	Water D_1 (Free e^-)	D_1 (Free h^+)
a	(TiO_2) ₄		
Vert			
Adia			
ΔE_{trap}		0.670	0.737
b			
Vert			
Adia			
ΔE_{trap}		0.597	1.064
c			
Vert			
Adia			
ΔE_{trap}		0.682	0.470
d			
Vert			

Adia



0.071



1.181

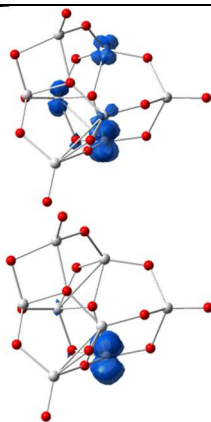
 ΔE_{trap}

	B3LYP S ₁ Exciton (e ⁻ -h ⁺ pair) (TiO ₂) ₈	Water D ₁ (Free e ⁻)	D ₁ (Free h ⁺)
a			
Vert			
Adia			
ΔE_{trap}		0.324	1.116
b			
Vert			
Adia			
ΔE_{trap}		0.693	1.162
c			
Vert			
Adia			
ΔE_{trap}		0.823	1.099

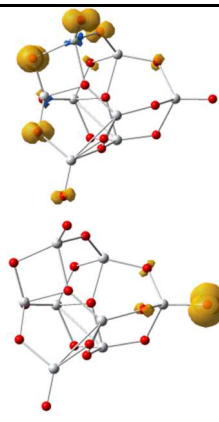
d

Vert

Adia

 ΔE_{trap} 

0.830



1.154

B3LYP
S₁ Exciton (e⁻-h⁺ pair)
(TiO₂)₁₆

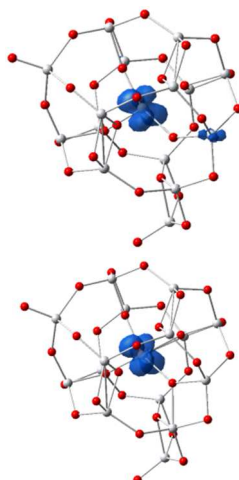
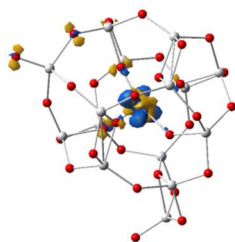
Water
D₁ (Free e⁻)

D₁ (Free h⁺)

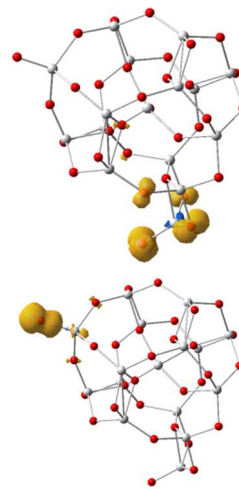
a

Vert

Adia

 ΔE_{trap} 

0.666

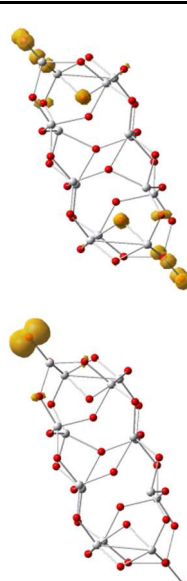
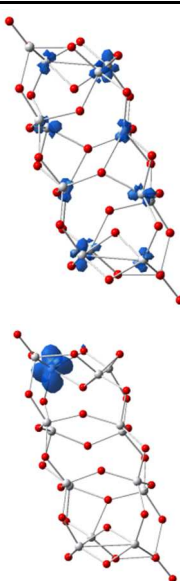
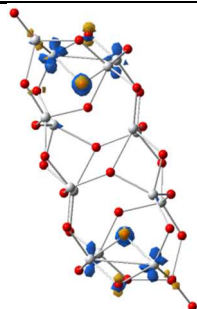


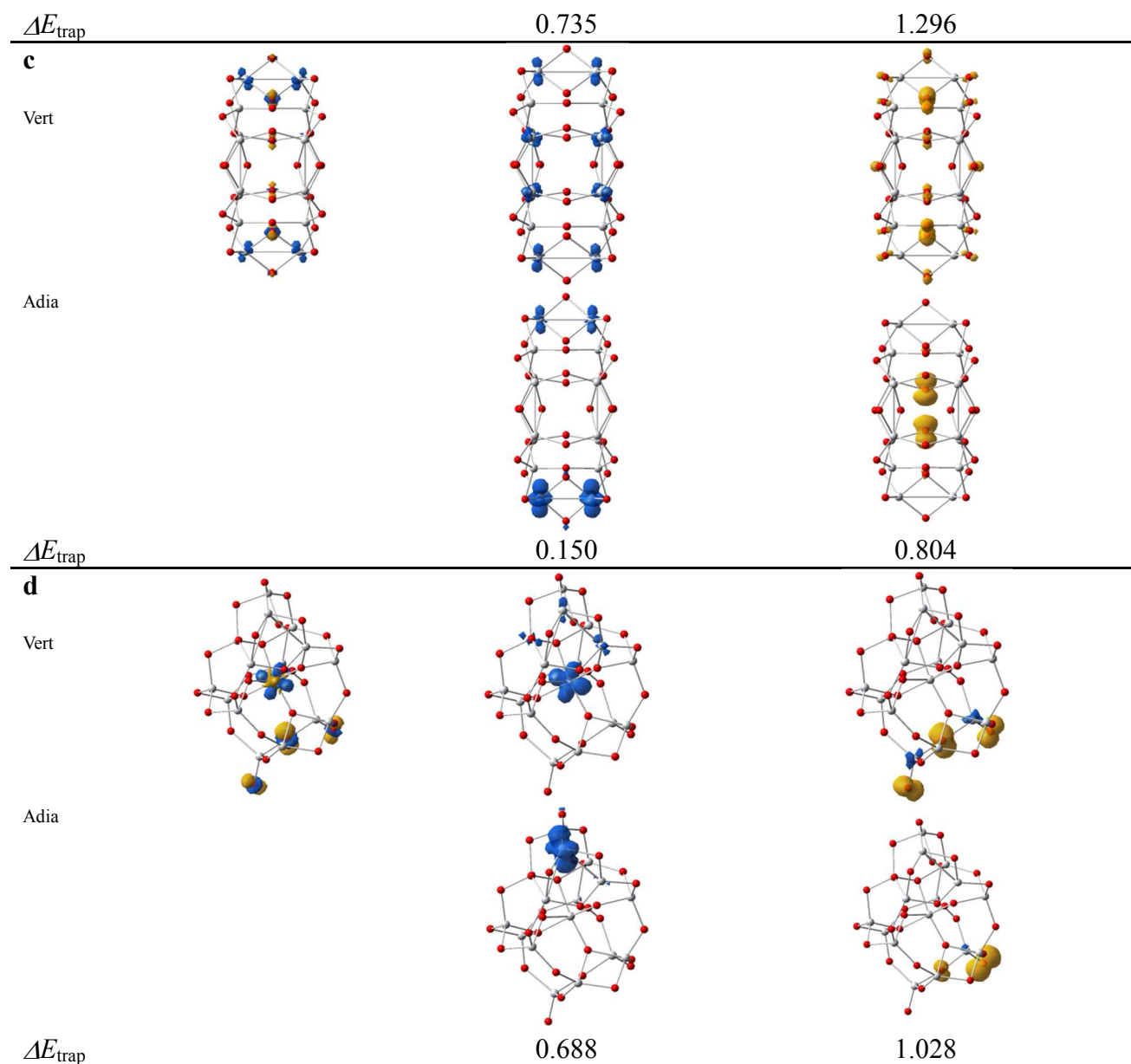
0.283

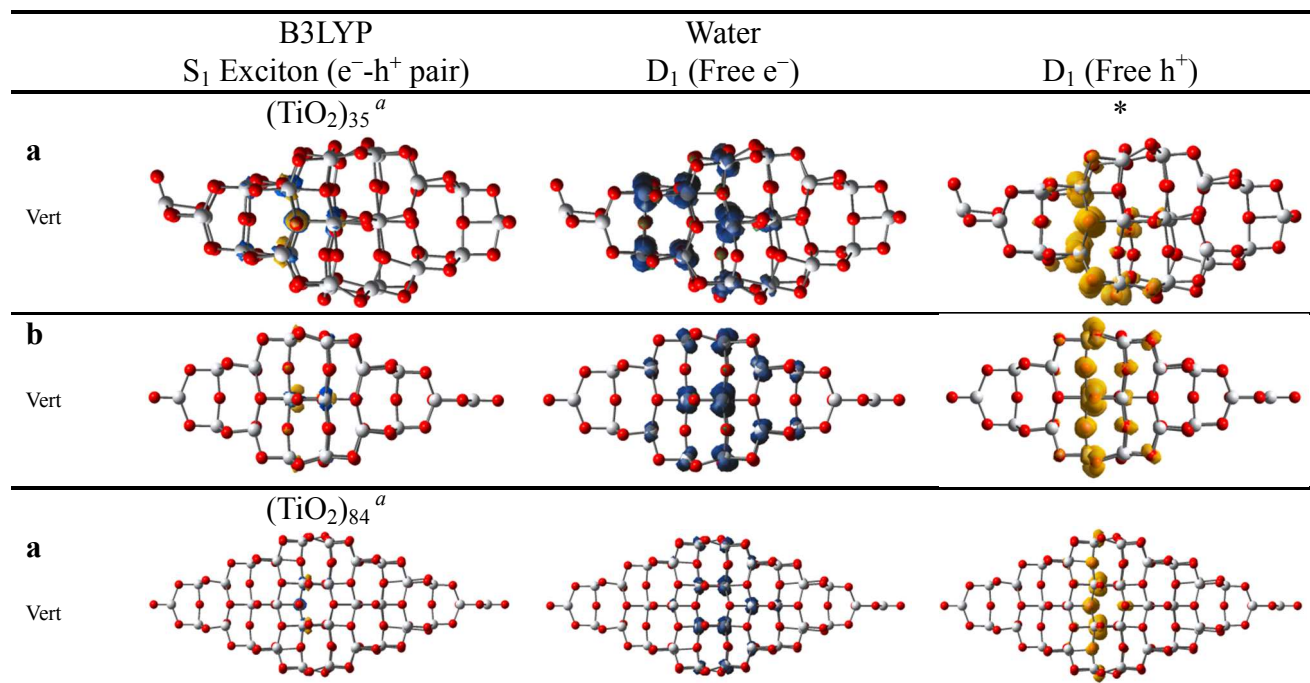
b

Vert

Adia







^a Calculated S₁ exciton pair, and free electron and hole distributions in (TiO₂)_{35a,35b,84} are drawn for isovalue of 0.004 and 0.001 e⁻au⁻³, respectively.

8. Optimized geometries of neutral ground state and relaxed cationic, anionic, and adiabatic S_1 exciton states of $(\text{TiO}_2)_n$ with $n = 4, 8, 16, 35, 84$ in vacuum at CAM-B3LYP/6-31G(d) level.

8.1. Optimized geometries of neutral, cationic, anionic, and adiabatic S_1 exciton state of $(\text{TiO}_2)_n$ with $n = 4, 8, 16, 35, 84$ in vacuum at CAM-B3LYP/6-31G(d) level.

8.1.1. Optimized geometries of $(\text{TiO}_2)_n$ with $n = 4, 8, 16, 35, 84$ in vacuum at CAM-B3LYP/6-31G(d) level.

$(\text{TiO}_2)_{4a}$

Ti	2.00870900	-0.00004100	0.61472100
Ti	-0.00001200	-1.39945300	-0.86886800
Ti	-0.00006400	1.39966500	-0.86852300
Ti	-2.00860000	-0.00011500	0.61497000
O	2.72984500	-0.00020100	2.03201800
O	1.65462500	-1.67444000	-0.29104200
O	1.65456600	1.67456700	-0.29063200
O	0.00004800	-0.00006300	0.51186700
O	-0.00010900	0.00024900	-2.02046200
O	-1.65463100	1.67450600	-0.29042700
O	-1.65456600	-1.67450200	-0.29083700
O	-2.72956100	-0.00030100	2.03235600

$(\text{TiO}_2)_{4b}$

Ti	-2.27340900	0.28628200	0.46769000
Ti	2.54573200	0.00701100	-0.33232700
O	0.84147000	-0.76807000	0.54834800
O	-3.60630000	1.10511700	0.18308000
O	3.87902000	-0.81131400	-0.04814400
O	1.47312800	-0.41891500	-1.88881700
Ti	0.36732000	0.91448000	1.19238600
O	-1.76244300	-1.16324700	-0.71548900
Ti	-0.09487400	-0.62229500	-1.05628200
O	-1.20103300	0.71184500	2.02446000
O	-0.56873100	1.06043200	-0.41242600

O	2.03454400	1.45619200	0.85115300
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(TiO₂)_{4c}

Ti	-1.59499300	0.00000000	0.88011500
Ti	1.59499300	0.00000000	0.88011500
O	0.00000000	0.00000000	1.76949500
O	-2.91530900	0.00000000	1.78399200
O	2.91530900	0.00000000	1.78399200
O	1.36566300	-1.47456500	-0.44866900
Ti	0.00000000	1.55038600	-1.45117500
O	0.00000000	0.00000000	-2.40068700
Ti	0.00000000	-1.55038600	-1.45117500
O	-1.36566300	-1.47456500	-0.44866900
O	-1.36566300	1.47456500	-0.44866900
O	1.36566300	1.47456500	-0.44866900

(TiO₂)_{4d}

Ti	-1.14904900	1.75126300	-0.86265400
Ti	0.16420500	0.04258700	-2.51392500
O	-0.63327100	-1.81780600	0.70354200
O	-1.62815900	0.40911400	-1.82746300
O	0.33521300	0.15192900	-4.09826600
O	0.96050100	-1.45206000	-1.64163100
Ti	-0.35308600	-0.16315200	1.70720400
O	0.44445500	1.69711600	-1.51007900
Ti	0.96016400	-1.87183000	0.05593100
O	-1.14961100	1.33135000	0.83487200
O	1.43923400	-0.52953800	1.02055700
O	-0.52386100	-0.27234900	3.29158100

$(\text{TiO}_2)_{8a}$

Ti	-3.20169600	-0.12941900	0.00002900
Ti	-0.92273400	1.32767500	-1.78297600
Ti	-0.92269700	1.32756600	1.78307400
Ti	0.75917800	2.68214100	0.00007300
Ti	0.92273200	-1.32767400	1.78297700
Ti	3.20169400	0.12941900	-0.00002800
Ti	0.92269500	-1.32756600	-1.78307400
Ti	-0.75918000	-2.68214100	-0.00007300
O	0.33869900	-1.13336300	-0.00003700
O	-2.57959800	0.94188900	-1.50516300
O	-4.77575200	-0.31944400	0.00003900
O	-0.33870000	1.13336300	0.00003800
O	-0.06067200	2.94650900	-1.61277200
O	-2.57956700	0.94179500	1.50527400
O	-0.06064000	2.94641200	1.61295100
O	2.28218500	1.86041700	0.00003500
O	0.00002700	-0.00007700	2.58778600
O	2.57959600	-0.94188900	1.50516400
O	4.77575000	0.31944400	-0.00003800
O	2.57956500	-0.94179500	-1.50527300
O	-0.00002900	0.00007700	-2.58778500
O	-2.28218700	-1.86041700	-0.00003400
O	0.06067000	-2.94650900	1.61277300
O	0.06063800	-2.94641200	-1.61295000

 $(\text{TiO}_2)_{8b}$

Ti	-1.39499900	-1.27096900	0.57591800
Ti	2.10165600	0.99831300	0.74436300

Ti	1.33085600	-2.47319700	0.06496800
O	1.25871300	-0.53026200	-0.06318400
Ti	-0.01791700	1.34916900	-1.41652200
Ti	2.46321500	-0.46590900	-1.57090200
Ti	-3.26004100	0.34028100	-0.82259100
O	2.00869100	0.49518300	2.38551500
O	-3.32308100	0.55174400	-2.54090000
O	-0.42020200	-2.68092400	-0.13504000
O	-3.41674100	2.03993100	-0.55385100
O	-0.72175800	-0.92941700	2.14226700
O	-3.77853900	3.50459400	-3.22430100
O	1.80460800	-2.50429200	1.71026300
O	-3.14441500	-1.15781100	0.36484500
O	1.06749600	-1.48399900	4.43272800
Ti	-2.91677700	2.45385000	-2.39242700
O	0.90511900	2.09513800	-0.01268800
O	-1.30661200	0.20560100	-0.64672800
O	1.24557700	0.46096800	-2.47372200
Ti	1.04008000	-1.12180700	2.88780900
O	2.47637400	-2.25277700	-1.39299100
O	3.42660500	0.59128100	-0.49298900
O	-0.95517400	2.47015900	-2.29748800

(TiO₂)_{8c}

Ti	-2.16514600	-1.53017700	0.82234700
Ti	3.08868100	1.19306300	-0.05973100
Ti	0.98537300	0.39559200	1.61430400
O	-2.60671500	-0.82193600	2.43777800
Ti	-3.13307400	1.03303800	-0.63364900
Ti	2.00322800	-1.30740500	-1.96341000

Ti	-1.85076200	0.81313000	2.18996000
O	3.97505800	2.46428000	-0.42263000
O	-4.44094400	1.62241600	-1.30765800
O	1.91825700	-2.94719400	-1.10330800
O	-3.25381200	-0.91901600	-0.34964400
O	2.66213900	0.85993000	1.75642000
O	-2.83106000	1.79037700	1.16141000
O	-1.00943100	-0.02853700	0.73087800
O	-1.02726500	-2.97665000	0.50239900
O	-1.57361300	1.22380500	-1.77943300
Ti	0.01758600	0.63087000	-1.48464000
O	-0.13073700	1.16207100	2.79421800
O	0.36272800	-1.15901400	-0.99082900
O	1.19417500	-1.48824700	1.53224100
Ti	0.68419900	-2.52603400	0.21176700
O	1.11462300	1.33850200	-0.14392200
O	3.21609400	-0.44247300	-1.13869800
O	1.11523600	0.12547100	-2.82703600

(TiO₂)_{8d}

Ti	3.21730700	0.09706800	-0.68049500
Ti	-1.11438300	0.07942200	-2.56415000
Ti	-1.22475800	-2.52411700	1.78022600
Ti	0.75477400	1.98723600	-1.65270400
O	4.80152000	0.07980000	-0.62713600
O	-0.64378300	0.67844600	1.16598000
O	0.16770800	-1.59091300	2.75745500
Ti	-2.37426000	0.19577700	0.48563500
Ti	0.70629900	-0.60409100	1.43230500
Ti	0.72418700	-1.66407700	-1.46739900

Ti	-1.09483600	2.60569100	1.12713000
O	2.45557100	1.67050100	-1.50916000
O	-2.42119000	0.08155700	-1.38537900
O	-0.78597700	3.42736700	2.45216900
O	-1.54258600	-4.05681400	2.06067300
O	-0.40564600	-1.57091500	-2.88783100
O	0.00540600	2.94925700	-0.41494300
O	2.39915600	-1.44866300	-1.63706400
O	-2.85255700	1.80629500	0.94088300
O	2.34784900	-0.17998300	1.02209400
O	0.24764900	0.15304100	-1.22633900
O	-2.63413300	-1.32012000	1.36027000
O	0.06457000	-2.01863000	0.25093200
O	-0.40542400	1.62427000	-3.09400600

(TiO₂)_{16a}

Ti	3.24786500	-1.57268400	1.44579900
Ti	2.33686400	0.35188400	-2.66458300
Ti	-0.34019800	1.52805700	-2.40022500
Ti	1.68642500	0.45832400	3.35561700
Ti	1.88626300	2.53054200	1.56404400
Ti	1.52859000	-5.20443000	-2.18554400
Ti	0.41474100	-0.44320000	-0.09028100
Ti	-1.36530700	-1.22438800	-2.69803200
Ti	-1.16842200	-2.95888900	1.76467900
Ti	1.32293800	-2.58193000	-3.19309600
Ti	1.77355300	-3.82337300	0.32133800
Ti	-2.95669600	-1.73462700	-0.43508200
Ti	-3.50920200	1.18870600	1.49266300

Ti	3.83201200	1.00755800	-0.40752100
Ti	-1.27893600	-0.67228400	3.31100600
Ti	-0.96157200	2.95303300	-0.01724300
O	-2.62726100	-3.10391600	0.75760100
O	4.35435300	-0.45365600	0.52777500
O	0.17980200	0.01774000	4.18466400
O	-3.60127500	-0.29731700	0.25847000
O	-2.56334300	0.42118100	3.00220200
O	0.50214000	3.50338800	0.98036000
O	-3.02110000	-1.84770300	-2.24296500
O	0.20410900	-6.06070000	-2.36923400
O	1.17049800	-3.35963600	-1.48099900
O	-2.45054400	2.66365500	0.79392800
O	-4.96119600	1.67060500	1.91356200
O	2.20296700	2.20254900	3.31972200
O	0.28430100	-3.95391300	1.36850500
O	1.89877600	-4.11359100	-3.74672000
O	-1.61357000	-2.47054400	3.43548200
O	2.21109400	-5.34145000	-0.39365900
O	3.34836500	-3.31153300	1.25775100
O	2.53931600	-1.22449100	-3.48208600
O	3.40182000	2.48368800	0.60382400
O	2.85822900	-0.87977400	3.09306000
O	4.02655500	1.00650800	-2.17487200
O	-0.41182200	-2.29930900	-3.73842600
O	-0.94453200	3.15505500	-1.82480800
O	2.14598200	0.51107300	-0.74846200
O	-1.14979000	-1.39639700	-0.75613300
O	-0.41553500	1.23370800	-0.43102600
O	1.68735000	-1.66952300	0.47775100

O	0.50377100	-0.46524100	-2.05644900
O	-0.63752700	-1.13937200	1.62022800
O	1.25019200	1.66099500	-3.27285100
O	-1.58324800	0.53457400	-3.18601000
O	1.21848700	0.78238700	1.60124500

(TiO₂)_{16b}

O	-0.11888700	-0.03160900	-0.01933900
Ti	-0.05115100	-0.09380500	1.92155100
O	1.87661400	0.01040300	2.27117700
O	0.40941200	-2.16030100	-2.20497000
Ti	0.89130600	-0.68218900	-1.25702700
O	-0.93132000	1.00437800	2.65498500
O	-0.39221000	-1.90213000	2.48979600
O	2.27884100	0.26552700	-1.97814900
O	4.43991200	-2.05124000	-1.88816700
Ti	3.64437200	-0.59218200	-1.15676400
O	2.27204400	-1.51650000	-0.24638500
O	0.34249100	-5.36822300	-1.99842100
O	0.13053900	-3.57498100	0.23867200
Ti	0.76732900	-3.74262900	-1.39890600
O	0.46584500	-4.94270700	2.84331900
O	4.34811900	-1.79024000	2.74692200
Ti	0.49666800	-3.29748900	1.98855300
O	2.26717100	-2.86226400	2.04713100
Ti	3.06098700	-1.01461300	1.62083600
O	4.17651700	-0.06751800	0.42415100
O	4.52448700	-3.50685300	0.62585800
Ti	4.14005400	-3.49103400	2.37802600
Ti	5.01748100	-6.17867700	2.54746400

O	3.24924400	-5.54843900	2.45824200
Ti	1.53671200	-6.23264000	2.28312300
O	5.44231900	-4.55308300	3.14697900
O	5.37539700	-7.76100500	3.35352700
Ti	4.89350300	-9.23911700	2.40558500
O	3.50596800	-10.18683300	3.12670600
O	1.34489800	-7.87006700	3.03672400
Ti	2.14043800	-9.32912500	2.30532100
O	3.51276500	-8.40480600	1.39494200
O	3.51763900	-7.05904300	-0.89857300
Ti	1.64475700	-6.43027200	-1.22946800
O	1.26032300	-6.41445300	0.52270000
O	1.43669100	-8.13106600	-1.59836400
O	1.60829300	-9.85378900	0.72440600
O	5.90369600	-9.88969800	1.16789600
O	3.90819600	-9.93171000	-1.12262000
Ti	2.72382300	-8.90669400	-0.47227900
O	6.17702000	-8.01917700	-1.34123900
O	5.65427200	-6.34632700	0.90988600
Ti	5.83596100	-9.82750200	-0.77299400
Ti	5.28814200	-6.62381800	-0.83999500
O	2.53556600	-4.37286700	-1.30968500
Ti	4.24809800	-3.68866600	-1.13456600
O	6.71613000	-10.92568500	-1.50642700
O	5.31896500	-4.97859900	-1.69476000

(TiO₂)_{16c}

Ti	-1.70843400	1.56923400	-2.27077000
Ti	-1.70843400	-1.56923400	-2.27077000
Ti	1.70843400	1.56923400	-2.27077000

Ti	1.70843400	-1.56923400	-2.27077000
Ti	-1.69107200	2.98025900	0.72225100
Ti	1.69107200	2.98025900	0.72225100
Ti	-1.69107200	-2.98025900	0.72225100
Ti	1.69107200	-2.98025900	0.72225100
Ti	-1.63463000	1.33214500	3.31663400
Ti	-1.63463000	-1.33214500	3.31663400
Ti	1.63463000	1.33214500	3.31663400
Ti	1.63463000	-1.33214500	3.31663400
Ti	1.37178300	4.52689700	-1.81209600
Ti	1.37178300	-4.52689700	-1.81209600
Ti	-1.37178300	4.52689700	-1.81209600
Ti	-1.37178300	-4.52689700	-1.81209600
O	2.15587500	-3.27645200	-2.84345000
O	2.15587500	3.27645200	-2.84345000
O	-2.15587500	-3.27645200	-2.84345000
O	-2.15587500	3.27645200	-2.84345000
O	-2.51877500	-2.54869700	2.26218800
O	-2.51877500	2.54869700	2.26218800
O	2.51877500	-2.54869700	2.26218800
O	2.51877500	2.54869700	2.26218800
O	2.13043600	-4.53365300	-0.17581800
O	-2.13043600	4.53365300	-0.17581800
O	2.13043600	4.53365300	-0.17581800
O	-2.13043600	-4.53365300	-0.17581800
O	-2.37690100	0.00000000	4.32052800
O	2.37690100	0.00000000	4.32052800
O	-2.47769200	0.00000000	-2.77585700
O	2.47769200	0.00000000	-2.77585700
O	0.00000000	-2.97140600	1.33549200

O	0.00000000	2.97140600	1.33549200
O	0.00000000	-1.31630700	-2.71904000
O	0.00000000	1.31630700	-2.71904000
O	1.92847600	-1.67004100	-0.49445600
O	-1.92847600	1.67004100	-0.49445600
O	1.92847600	1.67004100	-0.49445600
O	-1.92847600	-1.67004100	-0.49445600
O	0.00000000	-3.46808300	-1.26508600
O	0.00000000	3.46808300	-1.26508600
O	0.00000000	5.62676400	-2.35704400
O	0.00000000	-5.62676400	-2.35704400
O	-1.26248500	0.00000000	2.18753200
O	1.26248500	0.00000000	2.18753200
O	0.00000000	1.78750100	3.95672300
O	0.00000000	-1.78750100	3.95672300

(TiO₂)_{16d}

Ti	3.05479300	0.82080600	1.31450200
Ti	-0.34292000	4.29896300	1.97036800
Ti	-1.20988600	0.66879900	4.98265100
Ti	1.56674200	1.54911900	3.57269500
Ti	0.01910400	-0.20107600	0.56410400
Ti	-2.38125900	-1.13803300	-1.95121800
Ti	2.77142200	-2.29414000	0.25134400
Ti	-1.87235100	1.87058900	1.85049400
Ti	2.08981700	-2.15455600	-3.15683000
Ti	0.41246100	-3.54367400	1.22954100
Ti	0.93927900	2.54135800	-0.41193800
Ti	-0.76520800	-4.05643100	-2.03227800
Ti	-1.85712500	-1.69607700	3.05517100

Ti	0.38604800	0.68202500	-2.66291400
Ti	-0.34702700	3.25807700	4.60707100
Ti	-3.15307600	-0.58457600	0.70142800
O	-1.54849800	-0.98723700	-0.25904100
O	1.34441100	0.48122200	1.83450400
O	-0.65979100	-2.95654700	2.67747500
O	3.65408000	-0.81471300	0.93070000
O	3.02385300	-2.36284000	-1.40951200
O	-3.89367500	-0.79144400	-0.89259400
O	0.59174200	-3.10269300	-2.76784300
O	0.67829800	2.51585200	-2.13650000
O	-2.03740500	-0.97329100	4.70160200
O	3.27500300	1.46670200	3.00792100
O	-2.25031100	-2.76883700	-2.33325300
O	-0.97406600	2.12033300	6.01077900
O	2.93947300	-2.74858300	-4.36968100
O	1.51481900	-0.25385100	-3.50100700
O	2.21347600	-3.81537600	1.13411700
O	0.63499000	4.16634800	0.46659400
O	-1.01507300	-5.47519500	-2.71954900
O	-1.31132200	0.06835900	-2.83444800
O	2.64561200	2.10292400	0.11040700
O	-0.44412200	-4.22359800	-0.05578700
O	1.37304200	2.88807700	4.82074500
O	-3.35019600	-1.80708500	2.02580900
O	-1.82606200	1.88807700	3.76254800
O	-0.62502800	1.66900600	0.43958200
O	-3.35515700	1.17560600	1.20718900
O	-1.93833100	3.70460900	1.60573800
O	-0.51306800	4.84314400	3.77081200

O	0.48211700	0.37787400	4.44827800
O	-1.32555100	-0.19484900	2.07497300
O	0.91875700	-1.85062000	0.54134900
O	0.19967800	2.68473600	2.73247600
O	0.90520400	0.31859800	-0.90430900

(TiO₂)_{35a}

O	11.34857300	14.74619800	30.16583900
O	6.30144500	14.76076700	30.02902500
O	10.44497200	13.18003400	28.34725900
O	10.48037500	13.16097900	32.50683900
O	10.72200500	11.43537300	30.15515900
O	8.74489600	13.64465500	30.78979000
O	7.01689700	13.11614100	28.25874300
O	6.92034300	13.11753500	32.40338600
O	8.64884100	15.25105600	33.40856400
O	6.78293000	11.38003300	30.08515500
O	10.76508600	15.24036500	26.50576700
O	12.21963200	17.03274600	21.88961100
O	10.90977900	16.75777400	19.17088800
O	12.02570700	14.93608100	23.89682500
O	12.85258300	14.63290600	27.68798100
O	10.68986000	17.46314300	24.00038800
O	13.17715900	16.48188200	25.33837600
O	10.46747800	15.03165800	20.86374000
O	6.81620600	14.82042300	25.99751700
O	8.98470500	17.25119800	21.72171200
O	7.13795500	16.95566700	19.40440800
O	9.31648800	15.04066200	23.86724400

O	8.41252200	15.39586500	27.91563400
O	7.12558600	16.51012800	23.29437100
O	8.57666700	16.81429300	25.55329100
O	6.80884300	15.06144100	20.88246300
O	5.46654500	17.44822800	21.78788700
O	4.71581300	14.94758800	23.69520800
O	4.91668700	15.18163600	27.60818700
O	5.02932500	16.85988900	25.21431900
O	10.67377100	11.41449800	26.16085600
O	12.45859300	13.51048000	21.60855600
O	10.99270300	13.16645600	19.16630500
O	13.14654600	11.39086300	23.10995600
O	12.40168200	11.07793800	27.89209200
O	10.67689600	12.73787900	23.17240800
O	12.88001200	13.03222500	25.35503100
O	10.86106700	11.28332800	20.82597000
O	6.93591600	11.15795700	26.21735900
O	8.82170700	13.15753500	21.60101100
O	6.66204500	13.04123700	19.29333400
O	8.50497900	11.32832700	23.91011800
O	8.81401300	10.92912500	27.88259200
O	7.03164800	13.53743900	23.25559000
O	8.84960800	13.19586400	25.51081500
O	7.09125300	11.21261900	21.10276200
O	5.13202000	12.97585000	21.71081800
O	5.60796500	11.32118400	23.84478400
O	5.07566300	11.16522000	27.76361300
O	4.67444400	13.07075400	25.42188100
O	12.31652400	8.85628700	21.76237000
O	10.78597400	9.42332600	19.28597000

O	10.71662300	9.93942100	23.25901700
O	12.82708300	9.79549700	25.20372300
O	8.93187100	9.07608900	21.64410200
O	6.79252300	9.37396800	19.46938600
O	7.11621400	8.97824400	23.40089600
O	9.02212600	9.42556200	25.39923900
O	5.18227200	9.30021500	21.88662300
O	4.55088700	9.65906700	25.29217500
O	10.44011700	15.11533300	16.90590800
O	6.98052500	15.43681000	17.07562300
O	8.59596200	14.88683500	14.66088600
O	8.77212900	14.78362200	18.72951500
O	10.51156600	11.10593700	16.97764400
O	7.07211300	10.80980100	17.14005600
O	6.55670400	13.01070400	13.82041400
O	8.70553300	11.27657400	14.70604800
O	8.82803000	11.39056000	18.85368100
O	8.31212800	13.09444200	16.34193000
Ti	11.25728800	14.76910900	28.37528600
Ti	6.60848800	14.87810900	28.30040800
Ti	10.53939700	13.19048300	30.77721300
Ti	10.62938400	11.39184800	28.39020200
Ti	6.95789500	13.12840600	30.67340800
Ti	8.68055200	13.77572400	32.82940600
Ti	6.81481900	11.36482700	28.29180000
Ti	12.49700400	14.92112300	25.85788200
Ti	10.67370200	16.76459000	20.93690600
Ti	12.21504900	16.72630400	23.69149300
Ti	10.56186100	14.99004400	18.65982400
Ti	8.76036600	15.13178900	26.19249800

Ti	7.06952600	16.84599900	21.21955500
Ti	8.94950700	16.72857200	23.80401100
Ti	7.06591400	15.23150600	18.84067600
Ti	5.10593100	15.02960400	25.84591500
Ti	5.34756100	16.62528500	23.49478500
Ti	12.43495800	11.29802300	26.12390900
Ti	10.69958600	13.13994600	21.09860300
Ti	12.38874000	13.09592600	23.31379200
Ti	10.58820700	11.16197300	18.76722800
Ti	8.79049800	11.16513200	25.95532500
Ti	6.91201900	13.15201100	21.12416300
Ti	8.85101400	13.21062500	23.63467300
Ti	7.05901600	11.12276100	18.86572900
Ti	5.11493800	11.26694100	25.95149500
Ti	5.31755000	13.14772100	23.44723600
Ti	10.73381100	9.47192900	21.10328600
Ti	12.48877100	9.80515100	23.37034800
Ti	6.95019400	9.47054300	21.22811700
Ti	8.89164600	9.62964800	23.63317500
Ti	5.42386400	9.57257000	23.63774900
Ti	8.63863300	14.90339800	16.39171200
Ti	8.74951000	11.30301500	16.43286300
Ti	8.05804000	13.06178200	14.31860000

(TiO₂)_{35b}

Ti	17.21728000	17.00418000	43.79675000
Ti	17.05413000	15.25427000	46.13111000
Ti	20.77919000	17.00424000	43.79676000
Ti	18.99823000	17.20380000	41.34950000
Ti	20.94236000	15.25433000	46.13106000

Ti	17.21729000	20.98931000	43.79685000
Ti	16.99297000	18.99667000	46.12812000
Ti	18.99748000	18.99682000	38.84041000
Ti	20.77917000	20.98927000	43.79686000
Ti	18.99823000	20.78978000	41.34956000
Ti	21.00353000	18.99672000	46.12814000
Ti	17.05414000	22.73905000	46.13130000
Ti	20.94237000	22.73915000	46.13126000
Ti	15.36054000	15.35862000	48.51730000
Ti	17.00577000	17.21550000	53.23768000
Ti	15.25579000	17.05240000	50.90335000
Ti	18.99823000	15.31850000	48.63359000
Ti	20.99081000	17.21550000	53.23767000
Ti	18.99825000	16.99120000	50.90635000
Ti	22.63593000	15.35878000	48.51723000
Ti	22.74068000	17.05244000	50.90330000
Ti	15.32030000	18.99653000	48.40089000
Ti	17.00572000	20.77742000	53.23779000
Ti	15.25586000	20.94060000	50.90342000
Ti	17.20530000	18.99640000	55.68493000
Ti	18.99827000	18.99654000	48.51726000
Ti	20.99085000	20.77745000	53.23777000
Ti	18.99828000	21.00177000	50.90646000
Ti	20.79134000	18.99641000	55.68488000
Ti	22.67625000	18.99665000	48.40085000
Ti	22.74073000	20.94065000	50.90337000
Ti	15.36050000	22.63427000	48.51737000
Ti	18.99832000	22.67452000	48.63377000
Ti	22.63618000	22.63440000	48.51730000
Ti	18.99833000	18.99709000	58.19391000

O	18.99530000	18.99685000	37.22212000
O	17.07568000	17.06219000	46.00766000
O	17.13241000	15.04662000	48.38093000
O	16.94454000	15.23026000	44.30900000
O	17.27025000	16.81318000	41.99497000
O	15.30522000	14.83963000	46.71770000
O	20.92086000	17.06225000	46.00763000
O	18.99823000	17.20814000	43.91761000
O	20.86404000	15.04677000	48.38088000
O	21.05196000	15.23030000	44.30893000
O	18.99823000	17.23104000	39.55068000
O	20.72625000	16.81344000	41.99495000
O	18.99826000	14.84362000	46.58883000
O	22.69129000	14.83925000	46.71758000
O	17.07556000	20.93111000	46.00770000
O	17.09066000	18.99674000	48.24686000
O	16.79070000	18.99670000	44.20579000
O	17.27027000	21.18037000	41.99507000
O	15.17775000	18.99655000	46.59378000
O	18.99785000	18.99679000	41.51076000
O	20.92096000	20.93118000	46.00769000
O	18.99823000	20.78528000	43.91776000
O	20.90588000	18.99678000	48.24688000
O	21.20577000	18.99672000	44.20580000
O	18.99822000	20.76259000	39.55074000
O	20.72622000	21.18012000	41.99505000
O	18.99827000	18.99666000	46.57202000
O	22.81876000	18.99660000	46.59374000
O	17.13243000	22.94595000	48.38106000
O	16.94460000	22.76320000	44.30917000

O	15.30526000	23.15435000	46.71779000
O	20.86422000	22.94575000	48.38101000
O	21.05184000	22.76318000	44.30911000
O	18.99827000	23.14981000	46.58913000
O	22.69118000	23.15390000	46.71782000
O	14.84098000	15.30363000	50.31676000
O	16.81499000	17.26835000	55.03950000
O	15.23184000	16.94288000	52.72550000
O	15.04946000	17.13059000	48.65363000
O	17.06377000	17.07381000	51.02686000
O	18.99828000	15.17602000	50.44072000
O	21.18158000	17.26836000	55.03947000
O	18.99829000	16.78894000	52.82867000
O	18.99821000	17.08889000	48.78754000
O	20.93272000	17.07384000	51.02685000
O	23.15593000	15.30361000	50.31677000
O	22.76474000	16.94286000	52.72545000
O	22.94728000	17.13074000	48.65357000
O	14.84510000	18.99648000	50.44552000
O	16.81471000	20.72444000	55.03956000
O	15.23179000	21.05010000	52.72554000
O	17.23250000	18.99636000	57.48374000
O	17.20972000	18.99647000	53.11699000
O	15.04879000	20.86238000	48.65365000
O	17.06381000	20.91911000	51.02693000
O	18.99827000	18.99648000	50.46249000
O	21.18183000	20.72446000	55.03952000
O	18.99828000	21.20400000	52.82879000
O	20.76414000	18.99637000	57.48369000
O	20.78684000	18.99648000	53.11695000

O	18.99823000	20.90417000	48.78773000
O	20.93277000	20.91909000	51.02689000
O	18.99832000	18.99680000	55.52376000
O	23.15142000	18.99654000	50.44550000
O	22.76477000	21.05013000	52.72548000
O	22.94787000	20.86250000	48.65358000
O	14.84081000	22.68951000	50.31697000
O	18.99830000	22.81701000	50.44089000
O	23.15519000	22.68954000	50.31682000
O	18.99834000	18.99928000	59.81226000

(TiO₂)_{84a}

Ti	17.22287000	17.07534000	43.83230000
Ti	17.06650000	15.34986000	46.19808000
Ti	20.77379000	17.07554000	43.83243000
Ti	18.99842000	17.20064000	41.35711000
Ti	20.93026000	15.34987000	46.19803000
Ti	17.22287000	20.91795000	43.83235000
Ti	16.85775000	18.99661000	46.26068000
Ti	18.99666000	18.99670000	38.87121000
Ti	20.77377000	20.91776000	43.83249000
Ti	18.99841000	20.79269000	41.35712000
Ti	21.13897000	18.99662000	46.26086000
Ti	17.06647000	22.64338000	46.19815000
Ti	20.93024000	22.64338000	46.19810000
Ti	13.54957000	13.54673000	53.36872000
Ti	17.20496000	13.42554000	53.44122000
Ti	15.16232000	13.40503000	50.92749000
Ti	20.79183000	13.42567000	53.44116000

Ti	18.99837000	13.32249000	50.93801000
Ti	24.44748000	13.54700000	53.36836000
Ti	22.83444000	13.40496000	50.92742000
Ti	13.42798000	17.20326000	53.29550000
Ti	13.40669000	15.16051000	55.80911000
Ti	15.34876000	15.12403000	48.55860000
Ti	17.16408000	17.16213000	53.36829000
Ti	15.06463000	17.12888000	50.97909000
Ti	17.13065000	15.06264000	55.75744000
Ti	18.99840000	14.96653000	48.63895000
Ti	20.83280000	17.16213000	53.36824000
Ti	18.99840000	17.14621000	50.93509000
Ti	20.86615000	15.06267000	55.75740000
Ti	22.64801000	15.12403000	48.55855000
Ti	24.56901000	17.20325000	53.29537000
Ti	22.93219000	17.12886000	50.97904000
Ti	24.59005000	15.16052000	55.80901000
Ti	13.42796000	20.78985000	53.29552000
Ti	13.32412000	18.99653000	55.79856000
Ti	15.26960000	18.99660000	48.60111000
Ti	17.16407000	20.83098000	53.36833000
Ti	15.06463000	20.86428000	50.97913000
Ti	17.14806000	18.99653000	55.80136000
Ti	18.99833000	18.99660000	48.53254000
Ti	20.83279000	20.83098000	53.36828000
Ti	18.99838000	20.84696000	50.93513000
Ti	20.84875000	18.99653000	55.80134000
Ti	22.72712000	18.99662000	48.60119000
Ti	24.56901000	20.78994000	53.29539000
Ti	22.93217000	20.86434000	50.97907000

Ti	24.67263000	18.99656000	55.79845000
Ti	13.54951000	24.44633000	53.36878000
Ti	13.40668000	22.83255000	55.80919000
Ti	15.34873000	22.86916000	48.55867000
Ti	17.20495000	24.56755000	53.44131000
Ti	15.16229000	24.58813000	50.92759000
Ti	17.13063000	22.93042000	55.75752000
Ti	18.99837000	23.02666000	48.63903000
Ti	20.79181000	24.56743000	53.44124000
Ti	18.99834000	24.67069000	50.93811000
Ti	20.86613000	22.93041000	55.75748000
Ti	22.64799000	22.86921000	48.55863000
Ti	24.44755000	24.44616000	53.36841000
Ti	22.83441000	24.58827000	50.92754000
Ti	24.59005000	22.83260000	55.80909000
Ti	15.12582000	15.34687000	58.17791000
Ti	17.07732000	17.22102000	62.90411000
Ti	15.35174000	17.06459000	60.53845000
Ti	18.99843000	15.26782000	58.13522000
Ti	20.91969000	17.22099000	62.90409000
Ti	18.99848000	16.85586000	60.47570000
Ti	22.87103000	15.34689000	58.17784000
Ti	22.64522000	17.06460000	60.53837000
Ti	14.96842000	18.99650000	58.09754000
Ti	17.07730000	20.77190000	62.90415000
Ti	15.35173000	20.92837000	60.53848000
Ti	17.20256000	18.99644000	65.37938000
Ti	18.99843000	18.99652000	58.20402000
Ti	20.91969000	20.77195000	62.90413000
Ti	18.99847000	21.13712000	60.47575000

Ti	20.79456000	18.99645000	65.37928000
Ti	23.02844000	18.99652000	58.09747000
Ti	22.64521000	20.92839000	60.53841000
Ti	15.12581000	22.64614000	58.17799000
Ti	18.99841000	22.72522000	58.13530000
Ti	22.87100000	22.64616000	58.17791000
Ti	18.99857000	18.99644000	67.86529000
O	18.98991000	18.99672000	37.25400000
O	17.11742000	17.13473000	46.06449000
O	17.13422000	15.24979000	48.40555000
O	16.96244000	15.30568000	44.37882000
O	17.28117000	16.83438000	42.03727000
O	15.30236000	15.01307000	46.73950000
O	20.87928000	17.13475000	46.06453000
O	18.99833000	17.32910000	43.96199000
O	20.86255000	15.24986000	48.40551000
O	21.03427000	15.30583000	44.37873000
O	18.99867000	17.21557000	39.56107000
O	20.71576000	16.83530000	42.03726000
O	18.99838000	14.88797000	46.65174000
O	22.69438000	15.01309000	46.73942000
O	17.11740000	20.85850000	46.06453000
O	17.03275000	18.99661000	48.34199000
O	16.68529000	18.99663000	44.27298000
O	17.28116000	21.15898000	42.03732000
O	15.09193000	18.99660000	46.76504000
O	18.99710000	18.99666000	41.47771000
O	20.87928000	20.85850000	46.06457000
O	18.99832000	20.66421000	43.96201000
O	20.96393000	18.99661000	48.34202000

O	21.31143000	18.99664000	44.27313000
O	18.99866000	20.77781000	39.56108000
O	20.71574000	21.15808000	42.03731000
O	18.99833000	18.99662000	46.72297000
O	22.90477000	18.99662000	46.76511000
O	17.13419000	22.74343000	48.40562000
O	16.96242000	22.68760000	44.37889000
O	15.30233000	22.98015000	46.73956000
O	20.86254000	22.74337000	48.40557000
O	21.03425000	22.68747000	44.37880000
O	18.99836000	23.10526000	46.65183000
O	22.69436000	22.98016000	46.73949000
O	12.99929000	13.44026000	55.15525000
O	13.44163000	12.99957000	51.58163000
O	17.20248000	13.26668000	55.25411000
O	15.32018000	13.23683000	53.21983000
O	15.04191000	13.36321000	49.10533000
O	17.07151000	13.00071000	51.35919000
O	20.79459000	13.26667000	55.25402000
O	18.99839000	12.89516000	52.96843000
O	18.99842000	13.18214000	49.10821000
O	20.92534000	13.00055000	51.35926000
O	24.99734000	13.44013000	55.15507000
O	22.67674000	13.23827000	53.21958000
O	22.95470000	13.36321000	49.10521000
O	24.55500000	12.99909000	51.58142000
O	13.00193000	17.06952000	55.37717000
O	13.36498000	15.04045000	57.63143000
O	13.24398000	15.31794000	53.51754000
O	13.26854000	17.19953000	51.48274000

O	15.20203000	15.21130000	50.78685000
O	17.09374000	17.07579000	55.33601000
O	15.20076000	17.24310000	53.07312000
O	17.06554000	14.90187000	57.73996000
O	17.24250000	15.19853000	53.66309000
O	14.90376000	17.06353000	48.99653000
O	17.07767000	17.09224000	51.40037000
O	15.21309000	15.19939000	55.95008000
O	18.99844000	15.10237000	50.71650000
O	20.90305000	17.07583000	55.33598000
O	18.99841000	17.15225000	52.98456000
O	20.93138000	14.90186000	57.73991000
O	20.75380000	15.19860000	53.66315000
O	18.99835000	17.07700000	49.04084000
O	20.91916000	17.09221000	51.40037000
O	18.99842000	15.21507000	56.14325000
O	22.79497000	15.21129000	50.78669000
O	24.99476000	17.06957000	55.37711000
O	22.79616000	17.24251000	53.07317000
O	24.63188000	15.04034000	57.63128000
O	24.75433000	15.31806000	53.51717000
O	23.09301000	17.06359000	48.99649000
O	24.72826000	17.19985000	51.48257000
O	22.78371000	15.19960000	55.94991000
O	13.00194000	20.92353000	55.37723000
O	13.18394000	18.99650000	57.62831000
O	12.89686000	18.99655000	53.76813000
O	13.26854000	20.79356000	51.48277000
O	15.21619000	18.99658000	50.59295000
O	17.09374000	20.91727000	55.33605000

O	15.20075000	20.75009000	53.07317000
O	17.07875000	18.99652000	57.69559000
O	17.15615000	18.99655000	53.75190000
O	14.90375000	20.92965000	48.99656000
O	17.07765000	20.90091000	51.40040000
O	15.10404000	18.99652000	56.01978000
O	18.99842000	18.99659000	50.66080000
O	20.90303000	20.91724000	55.33602000
O	18.99840000	20.84084000	52.98458000
O	20.91808000	18.99652000	57.69557000
O	20.84093000	18.99656000	53.75179000
O	18.99834000	20.91623000	49.04088000
O	20.91915000	20.90096000	51.40041000
O	18.99840000	18.99652000	56.07587000
O	22.78039000	18.99660000	50.59302000
O	24.99472000	20.92354000	55.37717000
O	22.79616000	20.75074000	53.07322000
O	24.81289000	18.99653000	57.62821000
O	25.09999000	18.99660000	53.76803000
O	23.09299000	20.92962000	48.99652000
O	24.72824000	20.79330000	51.48260000
O	22.89273000	18.99654000	56.01975000
O	12.99934000	24.55282000	55.15533000
O	13.36497000	22.95259000	57.63150000
O	13.24376000	22.67514000	53.51758000
O	13.44162000	24.99356000	51.58174000
O	15.20198000	22.78186000	50.78690000
O	17.20240000	24.72639000	55.25420000
O	15.32014000	24.75606000	53.21990000
O	17.06551000	23.09116000	57.74005000

O	17.24257000	22.79457000	53.66318000
O	15.04189000	24.62997000	49.10543000
O	17.07147000	24.99245000	51.35930000
O	15.21308000	22.79363000	55.95013000
O	18.99842000	22.89081000	50.71659000
O	20.79463000	24.72641000	55.25411000
O	18.99837000	25.09797000	52.96855000
O	20.93136000	23.09119000	57.73999000
O	20.75367000	22.79451000	53.66324000
O	18.99839000	24.81105000	49.10831000
O	20.92531000	24.99263000	51.35937000
O	18.99840000	22.77803000	56.14333000
O	22.79497000	22.78193000	50.78675000
O	24.99697000	24.55299000	55.15511000
O	22.67676000	24.75461000	53.21965000
O	24.63184000	22.95274000	57.63134000
O	24.75454000	22.67512000	53.51721000
O	22.95465000	24.63001000	49.10532000
O	24.55493000	24.99389000	51.58156000
O	22.78370000	22.79344000	55.94995000
O	15.01502000	15.30048000	59.99708000
O	16.83661000	17.27910000	64.69922000
O	15.30761000	16.96057000	62.35773000
O	15.25170000	17.13234000	58.33091000
O	17.13662000	17.11559000	60.67199000
O	18.99849000	15.09010000	59.97132000
O	21.16035000	17.27911000	64.69919000
O	18.99851000	16.68336000	62.46343000
O	18.99844000	17.03099000	58.39451000
O	20.86035000	17.11561000	60.67197000

O	22.98194000	15.30049000	59.99699000
O	22.68938000	16.96058000	62.35765000
O	22.74518000	17.13235000	58.33085000
O	14.88981000	18.99648000	60.08468000
O	16.83659000	20.71378000	64.69926000
O	15.30760000	21.03235000	62.35777000
O	17.21744000	18.99641000	67.17543000
O	17.33095000	18.99646000	62.77465000
O	15.25169000	20.86067000	58.33095000
O	17.13661000	20.87738000	60.67202000
O	18.99846000	18.99650000	60.01357000
O	21.16035000	20.71379000	64.69923000
O	18.99850000	21.30958000	62.46348000
O	20.77967000	18.99642000	67.17533000
O	20.66601000	18.99647000	62.77456000
O	18.99843000	20.96204000	58.39454000
O	20.86034000	20.87738000	60.67200000
O	18.99857000	18.99646000	65.25883000
O	23.10711000	18.99650000	60.08462000
O	22.68937000	21.03237000	62.35769000
O	22.74517000	20.86069000	58.33089000
O	15.01498000	22.69248000	59.99716000
O	18.99846000	22.90289000	59.97140000
O	22.98192000	22.69252000	59.99706000
O	18.99857000	18.99652000	69.48236000

8.1.2. Optimized geometries of cationic $(\text{TiO}_2)_n$ with $n=4, 8, 16, 35, 84$ in vacuum at CAM-B3LYP/6-31G(d) level.

$(\text{TiO}_2)_{4a}$

Ti	1.99184900	-0.03943400	0.67070200
Ti	-0.00603700	-1.38952600	-0.92325500
Ti	0.12654700	1.45350300	-0.95315100
Ti	-2.01900200	-0.07542200	0.65460900
O	2.46248700	-0.02350900	2.16657500
O	1.54863500	-1.70083100	-0.22070700
O	1.72752700	1.63294200	-0.42024300
O	-0.02573000	0.12748000	0.42988200
O	0.02101900	0.09335800	-2.05829900
O	-1.81646600	1.74649900	-0.37811800
O	-1.60586800	-1.68493700	-0.25571700
O	-2.40471300	-0.14025200	2.17286300

$(\text{TiO}_2)_{4b}$

Ti	-2.21075900	0.34995200	0.41145100
Ti	2.56663900	0.15219200	-0.43594800
O	0.98305300	-0.86465200	0.58564700
O	-3.62112700	1.39321000	-0.01413400
O	3.90331900	-0.62059500	-0.18306600
O	1.35550000	-0.42840200	-1.88916700
Ti	0.43356900	0.73644300	1.31977900
O	-1.85468800	-1.11456800	-0.53524200
Ti	-0.03421000	-0.81823500	-0.95299000
O	-1.34297000	0.58441100	1.94794200
O	-0.47208500	0.91421500	-0.33218400
O	1.92818400	1.47354400	0.89154200

$(\text{TiO}_2)_{4c}$

Ti	-1.71146800	0.00000000	0.83065900
Ti	1.71146900	0.00000000	0.83064400
O	0.00001000	0.00000000	1.74857900
O	-3.06582200	0.00000000	1.64872900
O	3.06579600	0.00000000	1.64875600
O	1.35503800	-1.46446700	-0.39051800
Ti	-0.00000200	1.57537100	-1.42173500
O	-0.00000700	0.00000000	-2.30186600
Ti	-0.00000200	-1.57537200	-1.42173500
O	-1.35502500	-1.46447200	-0.39049800
O	-1.35502500	1.46447200	-0.39049800
O	1.35503800	1.46446700	-0.39051800

 $(\text{TiO}_2)_{4d}$

Ti	-1.17487200	1.79365300	-0.86546300
Ti	0.13911200	0.06594200	-2.43955800
O	-0.60198800	-1.84783900	0.73251200
O	-1.57787400	0.38387000	-1.83811600
O	0.34933500	0.15818800	-4.23347600
O	0.88000800	-1.32124500	-1.63733600
Ti	-0.35142700	-0.17511500	1.74518200
O	0.44741000	1.64424100	-1.52952100
Ti	0.96963200	-1.89871100	0.10445500
O	-1.13585900	1.32927800	0.76592800
O	1.44689000	-0.57585700	1.04795900
O	-0.52363300	-0.27978100	3.30710400

 $(\text{TiO}_2)_{8a}$

Ti	-3.23340400	-0.14734500	0.00002900
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Ti	-0.94117500	1.34468600	-1.79265100
Ti	-0.94113900	1.34457800	1.79275200
Ti	0.75775500	2.66690600	0.00007300
Ti	0.90090200	-1.33889200	1.78008700
Ti	3.13860600	0.11755800	-0.00002800
Ti	0.90086600	-1.33878500	-1.78018500
Ti	-0.78417700	-2.71406000	-0.00007400
O	0.32756800	-1.15213500	-0.00003800
O	-2.56811600	0.94646300	-1.48712500
O	-4.79454900	-0.33361000	0.00003900
O	-0.32778100	1.13568400	0.00003800
O	-0.04686900	2.96574400	-1.56720400
O	-2.56808600	0.94637100	1.48723600
O	-0.04683800	2.96565000	1.56738400
O	2.32718100	1.72522000	0.00003000
O	-0.01115400	-0.01738200	2.55094100
O	2.59325000	-0.88969100	1.42627200
O	4.92143600	0.39631500	-0.00003800
O	2.59322200	-0.88960400	-1.42637800
O	-0.01120700	-0.01722900	-2.55094100
O	-2.27373400	-1.87744800	-0.00003400
O	0.04372800	-2.91954400	1.63556400
O	0.04369500	-2.91944700	-1.63573900

(TiO₂)_{8b}

Ti	-1.37576200	-1.22246600	0.53974700
Ti	2.13736000	0.99623200	0.72708100
Ti	1.33721000	-2.47379200	0.04572600
O	1.27440400	-0.53672700	-0.06898500
Ti	-0.01650200	1.36115100	-1.42562100

Ti	2.46810700	-0.47040100	-1.61053400
Ti	-3.32508200	0.33875000	-0.84547700
O	1.99522200	0.39200700	2.39527000
O	-3.30617800	0.55134200	-2.54266400
O	-0.40389600	-2.63078600	-0.16636500
O	-3.44686500	2.01736400	-0.56479400
O	-0.60938400	-0.90400100	2.18828900
O	-3.81647800	3.49195200	-3.22707800
O	1.77277900	-2.44043400	1.75332800
O	-3.07562100	-1.20401800	0.38529500
O	0.98500600	-1.50468600	4.57494900
Ti	-2.93008600	2.47572500	-2.40683300
O	0.94512600	2.06537200	0.00850300
O	-1.31995500	0.23179000	-0.63876500
O	1.23299000	0.44052400	-2.47361300
Ti	1.03292700	-1.10691900	2.81533100
O	2.44539700	-2.26384600	-1.39585700
O	3.41357300	0.59926200	-0.51626000
O	-0.94155900	2.48145400	-2.27831800

(TiO₂)_{8c}

Ti	-2.19342300	-1.54977100	0.87856900
Ti	3.14215500	1.16073500	-0.03799300
Ti	1.01467400	0.41307800	1.64358800
O	-2.59009700	-0.82952300	2.49544700
Ti	-3.03150100	0.97866100	-0.58931600
Ti	2.02830700	-1.34050400	-2.00348200
Ti	-1.85641100	0.79671000	2.22206600
O	3.92158100	2.46541800	-0.45457800
O	-4.45657000	1.69036600	-1.42550400

O	1.93227700	-2.92630300	-1.10516400
O	-3.27996200	-0.85066700	-0.31460200
O	2.65330100	0.89891600	1.80379900
O	-2.85860100	1.73947600	1.07473000
O	-1.04855300	-0.06418600	0.76118300
O	-1.04111800	-2.92754600	0.52956600
O	-1.64025000	1.19784400	-1.70036300
Ti	0.07050800	0.62136500	-1.50885900
O	-0.18519900	1.16260200	2.79775000
O	0.35236100	-1.16473100	-1.05204900
O	1.22685100	-1.45616600	1.47043400
Ti	0.68637800	-2.51308100	0.19407300
O	1.13947100	1.26062300	-0.13738000
O	3.20378200	-0.46857800	-1.16845800
O	1.12485900	0.21112500	-2.82432300

(TiO₂)_{8d}

Ti	3.15596800	0.09858700	-0.67964300
Ti	-1.14437400	0.07957200	-2.56992300
Ti	-1.24884000	-2.52401000	1.79773800
Ti	0.75546700	1.98065600	-1.69051800
O	4.95429000	0.07523000	-0.55472000
O	-0.68249600	0.65977500	1.12107500
O	0.18654000	-1.50542200	2.74721200
Ti	-2.45503900	0.19218700	0.50458900
Ti	0.67734600	-0.56441900	1.43084100
Ti	0.71175000	-1.65889600	-1.46284600
Ti	-1.13023200	2.60262500	1.12222900
O	2.52208300	1.56145500	-1.49926300
O	-2.41148000	0.09928700	-1.37689200

O	-0.72693200	3.30705600	2.47384100
O	-1.54407900	-4.05687700	2.01450800
O	-0.42494700	-1.58990500	-2.84208200
O	0.03019900	2.88813300	-0.44904300
O	2.41735600	-1.37016300	-1.61445300
O	-2.88540500	1.79829200	0.98946800
O	2.38189800	-0.10553900	0.91612700
O	0.25269100	0.15809500	-1.25094300
O	-2.64974600	-1.33600700	1.36913600
O	0.07201400	-1.97777200	0.26098000
O	-0.42156700	1.64546400	-3.06827100

(TiO₂)_{16a}

Ti	3.27803700	-1.59297600	1.43965800
Ti	2.35367400	0.35810100	-2.68013300
Ti	-0.32946600	1.52721200	-2.40816600
Ti	1.69263000	0.45183800	3.34520900
Ti	1.88134600	2.54282400	1.56639600
Ti	1.54458200	-5.24571500	-2.20090600
Ti	0.46679100	-0.43576700	-0.08707500
Ti	-1.33122000	-1.22043900	-2.69698600
Ti	-1.17230900	-2.97508200	1.78635500
Ti	1.36395100	-2.62040800	-3.21532300
Ti	1.78541500	-3.85793100	0.30839500
Ti	-2.90570200	-1.70360700	-0.42442100
Ti	-3.49849200	1.17051600	1.49738200
Ti	3.85157700	1.01226300	-0.41625200
Ti	-1.28306500	-0.67203300	3.29562500
Ti	-0.97720100	2.92245700	-0.01865500

O	-2.62345300	-3.07392400	0.74947200
O	4.34835300	-0.45988000	0.50889300
O	0.15467300	0.00308300	4.14986200
O	-3.54295600	-0.19029700	0.31113000
O	-2.59654300	0.47662400	2.91122500
O	0.45743900	3.47916800	0.95899500
O	-3.01716200	-1.83921500	-2.18394300
O	0.14745300	-5.96529600	-2.35163400
O	1.25277700	-3.36571000	-1.49355400
O	-2.51881200	2.53596200	0.83361000
O	-5.10376800	1.67819300	1.95076700
O	2.20204500	2.18993500	3.31184500
O	0.26635600	-3.92708400	1.36483000
O	1.90879700	-4.14700200	-3.77108300
O	-1.61906200	-2.43156300	3.46436200
O	2.16687400	-5.38618900	-0.37218900
O	3.35453900	-3.32916300	1.22018500
O	2.54639700	-1.22655000	-3.46951500
O	3.37582600	2.47572300	0.60125400
O	2.85442800	-0.88008600	3.07123100
O	4.02982200	1.01048600	-2.18108300
O	-0.39672400	-2.30520000	-3.70887600
O	-0.95147200	3.16871700	-1.77887000
O	2.15767400	0.50638800	-0.76284900
O	-1.12517100	-1.39079500	-0.74439800
O	-0.42274800	1.23622900	-0.42768400
O	1.69162100	-1.65935500	0.49231800
O	0.49352100	-0.43048900	-2.05465000
O	-0.64666200	-1.14493800	1.63560100
O	1.24418800	1.67284200	-3.26898500

O	-1.56746200	0.53053700	-3.19303700
O	1.21494800	0.78892900	1.59063800
(TiO ₂) _{16b}			
O	-0.03992200	0.01224400	0.07764900
Ti	0.04491000	-0.07585100	1.90079500
O	1.84697400	-0.03229400	2.25136900
O	0.42052800	-2.10280900	-2.20188400
Ti	0.94427600	-0.66991300	-1.25118400
O	-0.91791900	1.20294600	2.75010300
O	-0.44359300	-1.69558300	2.42627500
O	2.32209800	0.24066100	-1.95785600
O	4.43125000	-2.10932300	-1.88011500
Ti	3.69631200	-0.64491000	-1.14622100
O	2.27800900	-1.56555600	-0.27632400
O	0.24767800	-5.31563500	-1.98138900
O	0.05349100	-3.52119500	0.22863300
Ti	0.72503400	-3.71643600	-1.40606500
O	0.31419600	-4.86859200	2.78776800
O	4.20529800	-1.92068100	2.79896900
Ti	0.39117900	-3.26331900	1.96653000
O	2.12970300	-2.90736700	2.00369200
Ti	3.08435800	-1.12838500	1.64246100
O	4.21382500	-0.20942700	0.47152900
O	4.42364100	-3.57260800	0.63007600
Ti	4.05208400	-3.68690200	2.38835500
Ti	4.94924700	-6.40315300	2.51088400
O	3.11440800	-5.51856300	2.44007200
Ti	1.42514400	-6.18157700	2.25157900
O	5.31024400	-4.70566600	3.12007700

O	5.74723000	-7.75002900	3.38895800
Ti	5.11117700	-9.28230600	2.59785200
O	3.59623500	-10.14147900	3.18207600
O	1.35796700	-7.79073000	3.03924200
Ti	2.38173200	-9.12540500	2.33440300
O	3.82206500	-8.09270600	1.84765400
O	3.44940800	-7.17838800	-0.81473100
Ti	1.55698300	-6.40619400	-1.25181100
O	1.15359700	-6.42838700	0.48353500
O	1.38067600	-8.05981300	-1.83167100
O	1.93917800	-9.60853500	0.68521000
O	5.83991100	-9.88773500	1.16674100
O	3.96802900	-9.93989600	-1.35415100
Ti	2.68802100	-8.94451300	-0.83625200
O	6.17117800	-8.03405000	-1.32118200
O	5.66421700	-6.33217000	0.90552800
Ti	5.84568500	-9.87593700	-0.78915800
Ti	5.25656000	-6.68722500	-0.81012000
O	2.46602800	-4.43169600	-1.31329900
Ti	4.19837900	-3.75235400	-1.13332300
O	6.79309100	-10.94675500	-1.45741300
O	5.22563800	-5.05516700	-1.69848300

(TiO₂)_{16c}

Ti	-1.76194100	1.53194100	-2.22948600
Ti	-1.76195200	-1.53104200	-2.23006300
Ti	1.76194100	1.53194100	-2.22948600
Ti	1.76195100	-1.53104200	-2.23006200
Ti	-1.71700000	2.94188900	0.74482000
Ti	1.71700000	2.94188800	0.74482000

Ti	-1.71700200	-2.94220100	0.74366600
Ti	1.71700300	-2.94220100	0.74366600
Ti	-1.64505200	1.33285400	3.38551900
Ti	-1.64505700	-1.33419700	3.38499200
Ti	1.64505200	1.33285400	3.38551900
Ti	1.64505700	-1.33419700	3.38499200
Ti	1.37367600	4.44788300	-1.87546800
Ti	1.37367600	-4.44712700	-1.87722900
Ti	-1.37367600	4.44788300	-1.87546800
Ti	-1.37367600	-4.44712700	-1.87722900
O	2.20641300	-3.16878900	-2.87252300
O	2.20642000	3.16994600	-2.87127500
O	-2.20641300	-3.16878800	-2.87252300
O	-2.20642000	3.16994700	-2.87127500
O	-2.50467600	-2.55397600	2.29431000
O	-2.50468500	2.55303800	2.29530500
O	2.50467600	-2.55397600	2.29431000
O	2.50468500	2.55303800	2.29530500
O	2.05274900	-4.47945100	-0.22770700
O	-2.05273800	4.47953400	-0.22592800
O	2.05273800	4.47953300	-0.22592800
O	-2.05274900	-4.47945100	-0.22770700
O	-2.36266600	-0.00086900	4.39297400
O	2.36266600	-0.00086900	4.39297400
O	-2.57226800	0.00054700	-2.73708800
O	2.57226800	0.00054700	-2.73708800
O	0.00000000	-2.91026600	1.24317200
O	0.00000000	2.90974200	1.24431300
O	0.00000000	-1.02700600	-2.66900300
O	0.00000000	1.02807500	-2.66865900

O	1.99140600	-1.62474300	-0.47812900
O	-1.99135200	1.62491400	-0.47750700
O	1.99135200	1.62491400	-0.47750700
O	-1.99140500	-1.62474300	-0.47812900
O	0.00000000	-3.29187900	-1.47666600
O	0.00000000	3.29247000	-1.47539000
O	0.00000000	5.54580700	-2.37038600
O	0.00000000	-5.54484600	-2.37259800
O	-1.27428700	-0.00045000	2.25288300
O	1.27428700	-0.00045000	2.25288300
O	0.00000000	1.79878500	3.97308700
O	0.00000000	-1.80028400	3.97242400

 $(\text{TiO}_2)_{16d}$

Ti	3.05302500	0.82304800	1.34081900
Ti	-0.34831300	4.31618800	1.98349700
Ti	-1.22894600	0.68083900	5.01167600
Ti	1.55834100	1.57385300	3.60615400
Ti	0.00771200	-0.17066800	0.61146400
Ti	-2.38213500	-1.10117800	-1.93800700
Ti	2.75504400	-2.26633100	0.22753500
Ti	-1.88474400	1.88399000	1.88030500
Ti	2.04055100	-2.16933800	-3.12051100
Ti	0.43742200	-3.53827900	1.22084800
Ti	0.93543100	2.55867000	-0.40540400
Ti	-0.77487900	-4.06847600	-2.02171800
Ti	-1.85569600	-1.70573700	3.06061400
Ti	0.40234100	0.68362600	-2.63334300
Ti	-0.35598700	3.27962700	4.63021700
Ti	-3.16276100	-0.58049400	0.71076800

O	-1.55270100	-0.96698300	-0.25747800
O	1.34529000	0.45197200	1.85496500
O	-0.62606200	-2.94415000	2.63420700
O	3.63077500	-0.83608700	0.92227500
O	2.95975300	-2.30945100	-1.49703500
O	-3.88754200	-0.79952100	-0.90027400
O	0.69999200	-3.20113100	-2.90843900
O	0.68632000	2.48645000	-2.15241200
O	-2.03027500	-0.98046000	4.68475100
O	3.26394600	1.48088600	3.01193600
O	-2.14677000	-2.72897900	-2.34184000
O	-0.98486700	2.14518000	6.01346800
O	2.98019000	-2.86361100	-4.49521600
O	1.51019000	-0.40117600	-3.45549100
O	2.25450000	-3.77259600	1.11061000
O	0.63378300	4.15189400	0.46505100
O	-1.12471500	-5.46441800	-2.66833800
O	-1.28839000	0.12292700	-2.78833600
O	2.62086900	2.08757800	0.13683700
O	-0.39358300	-4.21599300	-0.09919800
O	1.36610200	2.90290000	4.83961100
O	-3.34034000	-1.80812700	2.02504300
O	-1.84978800	1.88075200	3.77300500
O	-0.60406200	1.66613800	0.46004200
O	-3.34970000	1.17585900	1.21096000
O	-1.93379200	3.70491100	1.61095000
O	-0.52277100	4.85120700	3.76485000
O	0.45563900	0.40396100	4.45793600
O	-1.32802200	-0.19321600	2.07627100
O	0.92299300	-1.85176200	0.50883900

O	0.18870800	2.68784000	2.75110200
O	0.88563500	0.30375200	-0.90930400

8.1.3. Optimized geometries of anionic $(\text{TiO}_2)_n$ with $n=4, 8, 16, 35, 84$ in vacuum at CAM-B3LYP/6-31G(d) level. $(\text{TiO}_2)_{4a}$

Ti	2.00159000	-0.00221000	0.63697700
Ti	-0.00001600	-1.30738000	-0.84276000
Ti	-0.00005600	1.48051000	-0.81061000
Ti	-2.00147700	-0.00228200	0.63722600
O	2.90868800	0.00121700	1.98260300
O	1.70364400	-1.63344100	-0.32399200
O	1.79284000	1.58170400	-0.32376100
O	0.00005300	-0.00097900	0.64672800
O	-0.00011100	-0.06652000	-2.05291700
O	-1.79289300	1.58164600	-0.32353500
O	-1.70360000	-1.63350400	-0.32378000
O	-2.90841100	0.00111000	1.98296300

 $(\text{TiO}_2)_{4b}$

Ti	-2.26017600	0.34706300	0.40966800
Ti	2.52902500	-0.06696800	-0.29191700
O	0.88593400	-0.83506800	0.55768300
O	-3.69521900	1.07241700	0.18754100
O	3.95791400	-0.81198700	-0.09676700
O	1.47242900	-0.38488300	-1.88619600
Ti	0.38953500	0.98835700	1.29955400
O	-1.75506300	-1.17239400	-0.68341900
Ti	-0.07771300	-0.56415100	-0.97323300
O	-1.31225800	0.65505500	1.99120200
O	-0.62157800	1.10451700	-0.45766300
O	2.12159500	1.42555900	0.75717800

 $(\text{TiO}_2)_{4c}$

Ti	-1.61005600	0.00000000	0.86020600
Ti	1.61005600	0.00000000	0.86020600
O	0.00000000	0.00000000	1.75054000
O	-2.94221100	0.00000000	1.78705400
O	2.94221100	0.00000000	1.78705400
O	1.44091100	-1.46983400	-0.42038000
Ti	0.00000000	1.38561800	-1.38873100
O	0.00000000	0.00000000	-2.58607900
Ti	0.00000000	-1.38561800	-1.38873100
O	-1.44091100	-1.46983400	-0.42038000
O	-1.44091100	1.46983400	-0.42038000
O	1.44091100	1.46983400	-0.42038000

 $(\text{TiO}_2)_{4d}$

Ti	-0.85601100	1.23188400	-0.66737900
Ti	0.21268200	0.03802600	-2.81307700
O	-0.79240300	-1.63566300	0.78902800
O	-1.51701200	0.19784400	-1.91905200
O	0.33964800	0.22603100	-4.42096700
O	0.98308000	-1.41830900	-1.93511200
Ti	-0.40154900	-0.15858300	2.00635700
O	0.60348500	1.51514200	-1.59576600
Ti	0.66711900	-1.35245900	-0.13934400
O	-1.17190700	1.29777800	1.12839800
O	1.32814900	-0.31846200	1.11234300
O	-0.52854600	-0.34660800	3.61424200

 $(\text{TiO}_2)_{8a}$

Ti	-3.22341400	-0.11618900	-0.00857600
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Ti	-0.92139000	1.27610900	-1.81275700
Ti	-0.91905100	1.28062300	1.76257300
Ti	0.75126500	2.63360100	-0.00660600
Ti	0.94435000	-1.34234500	1.76216000
Ti	3.21759100	0.12617600	0.02011300
Ti	0.99401700	-1.32101500	-1.86438800
Ti	-0.76245400	-2.61693400	0.01456600
O	0.37678900	-1.13893200	0.04324600
O	-2.60722100	0.91496700	-1.52181700
O	-4.81734800	-0.28573700	-0.00278900
O	-0.33437800	1.10023200	-0.00836900
O	-0.01839700	2.91800200	-1.62846500
O	-2.59873200	0.94256700	1.51697300
O	-0.08142200	2.92110700	1.61369700
O	2.30732100	1.87927500	0.03997200
O	-0.00509900	-0.01276100	2.61256400
O	2.62861300	-0.95862400	1.53213400
O	4.80717600	0.33792100	0.04389500
O	2.66730900	-0.82211400	-1.51469900
O	-0.09059000	0.04367100	-2.71667100
O	-2.33992300	-1.81047500	0.03489900
O	0.10436500	-2.96434200	1.64402900
O	-0.07939600	-2.98478100	-1.55567600

(TiO₂)_{8b}

Ti	-1.20660700	-1.22252000	0.50901500
Ti	2.01133800	0.90472100	0.71407800
Ti	1.36001900	-2.52004100	0.13219400
O	1.09534700	-0.63477300	0.01084200
Ti	-0.02127500	1.49829400	-1.51055800

Ti	2.34672600	-0.53092800	-1.61343300
Ti	-3.14872400	0.33968200	-0.85332300
O	2.02749300	0.46021000	2.41767900
O	-3.32270300	0.57803600	-2.57918800
O	-0.42090400	-2.77244300	-0.08419200
O	-3.42097300	2.03661200	-0.55296600
O	-0.67568200	-0.95595100	2.14379000
O	-3.87523100	3.53799700	-3.19966000
O	1.85715400	-2.56809500	1.79811700
O	-2.99452600	-1.14703200	0.29750700
O	1.11222900	-1.46268500	4.46957100
Ti	-2.96536100	2.48352800	-2.39208500
O	0.88756800	2.13045000	-0.08231500
O	-1.25080500	0.28504200	-0.74075800
O	1.17370600	0.57683500	-2.51798500
Ti	1.10141600	-1.14293700	2.89871700
O	2.48801200	-2.38795700	-1.27053000
O	3.36437000	0.57401200	-0.34991200
O	-1.04985200	2.62479100	-2.37225200

(TiO₂)_{8c}

Ti	-2.20413900	-1.55409100	0.81545500
Ti	3.12998100	1.14824200	-0.12381000
Ti	1.06977700	0.41312500	1.63835300
O	-2.59847600	-0.82992800	2.44838500
Ti	-3.13709500	1.01507100	-0.63905600
Ti	2.09019000	-1.26783500	-1.92378900
Ti	-1.81216400	0.78983900	2.14059900
O	3.97470000	2.47087200	-0.46999400
O	-4.45634800	1.62934500	-1.30372300

O	1.96009700	-2.92083000	-0.89604000
O	-3.32472600	-0.92960300	-0.34538600
O	2.74946300	0.84146700	1.75744100
O	-2.82812100	1.79310700	1.15232300
O	-1.03369200	-0.06826500	0.68448500
O	-1.12113300	-3.01191700	0.56579400
O	-1.61289600	1.24056400	-1.76816800
Ti	-0.02988100	0.54632000	-1.42481500
O	-0.14106300	1.18138300	2.79149600
O	0.13866500	-1.31719200	-1.21472000
O	1.16472600	-1.42497600	1.49107300
Ti	0.59716500	-2.44658400	0.14106100
O	1.12743600	1.24325700	-0.08417000
O	3.45054200	-0.35391700	-1.19884500
O	1.16181000	0.31840900	-2.68481300

(TiO₂)_{8d}

Ti	3.24075500	0.06864500	-0.72642500
Ti	-1.06794500	0.04395500	-2.41331200
Ti	-1.21647800	-2.51143700	1.71880800
Ti	0.77613200	1.92127900	-1.56479200
O	4.83837900	0.09315700	-0.60098700
O	-0.71415200	0.71467800	1.19920500
O	0.14898600	-1.51956900	2.63091900
Ti	-2.42826200	0.21797700	0.55254700
Ti	0.65314800	-0.61779600	1.20836100
Ti	0.86659600	-1.80417000	-1.58327100
Ti	-1.13455500	2.62995100	1.12066400
O	2.50419400	1.68277300	-1.52084300
O	-2.46220100	0.04591700	-1.27446400

O	-0.87776700	3.52981800	2.42330400
O	-1.50951600	-4.04115100	2.12225000
O	-0.50927200	-1.51831700	-2.95287400
O	0.00117700	2.97060200	-0.37219100
O	2.58422700	-1.46326600	-1.68804800
O	-2.90254800	1.87342000	0.94616400
O	2.32781200	-0.17691000	0.96089500
O	0.30257300	0.12710900	-1.10647600
O	-2.67697700	-1.30985000	1.43065700
O	-0.01713100	-2.09516700	0.19316800
O	-0.33471000	1.59575500	-3.01411300

(TiO₂)_{16a}

Ti	3.32997100	-1.61278200	1.52425000
Ti	2.32132100	0.35922700	-2.67728400
Ti	-0.33826100	1.57569800	-2.47563900
Ti	1.67300400	0.44856800	3.33561900
Ti	1.86291000	2.49621500	1.52026800
Ti	1.45422500	-5.06633700	-2.11595100
Ti	0.43159800	-0.48136800	-0.08641200
Ti	-1.42120000	-1.14989300	-2.72539100
Ti	-1.17299200	-3.03056500	1.77622400
Ti	1.23096700	-2.45293500	-3.11996400
Ti	1.82359400	-3.76253600	0.42144900
Ti	-2.96166200	-1.74075100	-0.45863300
Ti	-3.48118300	1.14504900	1.48473000
Ti	3.84300400	0.93341400	-0.41334500
Ti	-1.27565000	-0.75118700	3.30608300
Ti	-0.94635300	2.93101200	-0.09416100

O	-2.59325500	-3.15210700	0.70785100
O	4.42487300	-0.49059900	0.55335000
O	0.18073700	-0.05429800	4.18570300
O	-3.67401200	-0.34610400	0.29093800
O	-2.54996800	0.36674100	2.99754200
O	0.51097400	3.51039100	0.92776700
O	-3.09404300	-1.80011900	-2.26328400
O	0.20147300	-6.04919900	-2.29080300
O	1.08256300	-3.25572100	-1.39231000
O	-2.42747500	2.59332900	0.75000300
O	-4.91441000	1.68341700	1.93907400
O	2.16475400	2.20846400	3.29582700
O	0.31669100	-4.00851600	1.42400600
O	1.81946400	-4.00287100	-3.66887100
O	-1.65509400	-2.54656500	3.45209600
O	2.30227700	-5.22800000	-0.41883500
O	3.41578100	-3.37167300	1.41457700
O	2.53251900	-1.19774400	-3.53031200
O	3.39526600	2.43243500	0.58674100
O	2.92099200	-0.81517400	3.15244000
O	4.05015300	0.98565400	-2.17963300
O	-0.49487600	-2.27713500	-3.74730000
O	-0.96776600	3.21033000	-1.89772100
O	2.18841400	0.41157100	-0.76798800
O	-1.22659300	-1.31834100	-0.80687600
O	-0.35182700	1.29789200	-0.57180800
O	1.81567700	-1.74154500	0.60955100
O	0.48768500	-0.45444100	-2.18948700
O	-0.64442700	-1.24919800	1.64750000
O	1.28884900	1.72295000	-3.28933400

O	-1.61693500	0.59456500	-3.26027400
O	1.19452900	0.76211800	1.59299300
(TiO ₂) _{16b}			
O	-0.23035800	0.00716700	0.09552000
Ti	-0.05803400	-0.08496100	1.97247600
O	1.87544600	0.01625000	2.24497800
O	0.37995200	-2.25583900	-2.26406200
Ti	0.74741300	-0.61659500	-1.24981500
O	-0.90419600	1.02269700	2.76193600
O	-0.37051900	-1.90064400	2.58396500
O	2.34523400	0.20917300	-2.08143700
O	4.45751700	-2.14068400	-1.94489100
Ti	3.55259200	-0.68161500	-1.20748300
O	2.26925000	-1.60512900	-0.24218500
O	0.35700600	-5.32406600	-1.94858600
O	0.10188800	-3.52182700	0.29874500
Ti	0.81030000	-3.65315100	-1.34069400
O	0.45656300	-4.96035100	2.85624300
O	4.39748200	-1.77045800	2.65900600
Ti	0.50459900	-3.28335600	2.02673200
O	2.28981200	-2.89301100	2.09104800
Ti	3.04720800	-0.99813000	1.53558000
O	4.10310600	-0.03125300	0.37133500
O	4.55278200	-3.55376200	0.61360000
Ti	4.14455100	-3.45973000	2.35381800
Ti	5.00737000	-6.17046900	2.57114700
O	3.23966200	-5.58881600	2.46021700
Ti	1.52488400	-6.23366800	2.27211000
O	5.42238900	-4.56121600	3.18866000

O	5.35601900	-7.77590100	3.38070100
Ti	4.86561900	-9.22517900	2.40206700
O	3.47513000	-10.18877000	3.10287700
O	1.30628900	-7.88787500	3.01930000
Ti	2.12431400	-9.30793900	2.25543900
O	3.50982400	-8.38947300	1.38865700
O	3.56901000	-7.04212000	-0.86683600
Ti	1.66516700	-6.34139300	-1.24085200
O	1.26425900	-6.42415200	0.51232900
O	1.50775500	-8.07158900	-1.67632500
O	1.58765900	-9.80723300	0.66885700
O	5.89355200	-9.90252900	1.18242000
O	3.91248600	-9.90474900	-1.14889600
Ti	2.72801400	-8.84328300	-0.52289400
O	6.22526600	-8.04230800	-1.30435200
O	5.70210800	-6.35201000	0.95364300
Ti	5.82117000	-9.82424500	-0.75686800
Ti	5.33376400	-6.62775500	-0.80029500
O	2.58111200	-4.42306700	-1.32807500
Ti	4.28668600	-3.72661900	-1.15633200
O	6.69705800	-10.94377500	-1.48534700
O	5.39928300	-5.02595500	-1.69180000

(TiO₂)_{16c}

Ti	-1.70742200	1.56595900	-2.27392900
Ti	-1.70741100	-1.56597700	-2.27395300
Ti	1.70739100	1.56596100	-2.27392900
Ti	1.70738200	-1.56597600	-2.27395500
Ti	-1.68170100	2.96483100	0.70676800
Ti	1.68168000	2.96484100	0.70675600

Ti	-1.68169300	-2.96483400	0.70676400
Ti	1.68167600	-2.96484000	0.70675200
Ti	-1.62320900	1.33232500	3.28619800
Ti	-1.62320600	-1.33231600	3.28619200
Ti	1.62319700	1.33232700	3.28618300
Ti	1.62319700	-1.33231400	3.28617600
Ti	1.35762400	4.49247300	-1.79403300
Ti	1.35763100	-4.49247200	-1.79403400
Ti	-1.35764400	4.49246800	-1.79403100
Ti	-1.35764300	-4.49246800	-1.79403100
O	2.16942900	-3.24911700	-2.85812400
O	2.16942100	3.24910700	-2.85810800
O	-2.16943900	-3.24910800	-2.85813100
O	-2.16943300	3.24909000	-2.85811800
O	-2.52727100	-2.54712700	2.26604100
O	-2.52726900	2.54714700	2.26605700
O	2.52726000	-2.54712800	2.26602000
O	2.52725300	2.54715400	2.26603500
O	2.14010500	-4.52296500	-0.13646800
O	-2.14009900	4.52295100	-0.13644800
O	2.14010500	4.52296400	-0.13647200
O	-2.14009800	-4.52295700	-0.13644800
O	-2.38475600	-0.00000100	4.28862200
O	2.38475400	0.00000300	4.28860000
O	-2.48524200	-0.00001000	-2.79837700
O	2.48521100	-0.00000600	-2.79837600
O	-0.00000500	-2.92026300	1.36836800
O	-0.00000600	2.92024800	1.36834900
O	-0.00001000	-1.31197500	-2.73815100
O	-0.00001000	1.31197900	-2.73809800

O	1.96117100	-1.65180400	-0.49299000
O	-1.96121200	1.65178500	-0.49296300
O	1.96120000	1.65179100	-0.49297000
O	-1.96118400	-1.65180300	-0.49298200
O	0.00005600	-3.41308700	-1.21846800
O	0.00007200	3.41310600	-1.21845600
O	0.00009400	5.62850400	-2.34845500
O	0.00007200	-5.62849900	-2.34845900
O	-1.25471500	0.00000900	2.15799300
O	1.25469700	0.00001100	2.15798000
O	-0.00000100	1.78256300	3.97376500
O	0.00000100	-1.78254800	3.97376700

 $(\text{TiO}_2)_{16d}$

Ti	3.00939100	0.81186500	1.35175800
Ti	-0.30208100	4.27250000	1.98707200
Ti	-1.19561500	0.66745200	4.94243200
Ti	1.53880000	1.62543500	3.65734400
Ti	0.03424200	-0.15954200	0.58626600
Ti	-2.36451600	-1.14027400	-1.91076800
Ti	2.74658100	-2.26325800	0.24483600
Ti	-1.88029400	1.91293200	1.87644200
Ti	2.09030300	-2.13942300	-3.15122100
Ti	0.40724500	-3.53286500	1.19773500
Ti	0.93161600	2.58654900	-0.41217800
Ti	-0.75367500	-4.06014600	-2.04308300
Ti	-1.84337600	-1.70026300	3.04874500
Ti	0.37631200	0.67257400	-2.63543100
Ti	-0.40543200	3.27578400	4.68024700
Ti	-3.14399800	-0.57029600	0.72452600

O	-1.55001200	-0.99545200	-0.23631100
O	1.32583500	0.39859400	1.84317200
O	-0.66204000	-2.99391400	2.65458100
O	3.65758500	-0.82909300	0.94813800
O	3.03403500	-2.34456400	-1.42222400
O	-3.88986300	-0.78918900	-0.88676400
O	0.62570600	-3.16045500	-2.80851700
O	0.66612500	2.49223300	-2.16730500
O	-2.02151200	-1.01100400	4.69876100
O	3.25263700	1.50337200	3.00137600
O	-2.22470600	-2.77694200	-2.32857300
O	-1.01194700	2.03164600	6.05770900
O	2.98296900	-2.69354400	-4.36349400
O	1.49151700	-0.26617400	-3.51845300
O	2.21795500	-3.79760100	1.13862200
O	0.66603000	4.19064300	0.37768500
O	-1.05697000	-5.47823400	-2.73112700
O	-1.34069900	0.07752700	-2.82139000
O	2.62051100	2.09390200	0.14107900
O	-0.43053300	-4.27099900	-0.08356100
O	1.42177400	2.89143900	4.88157200
O	-3.36217200	-1.80128400	2.04646900
O	-1.89055000	1.90429300	3.76739400
O	-0.60502600	1.67515200	0.43206700
O	-3.36433000	1.17283500	1.20722900
O	-1.97041300	3.68947800	1.63695300
O	-0.36017800	4.99249800	3.57316200
O	0.49840100	0.34950700	4.45238500
O	-1.33496000	-0.20278000	2.08464900
O	0.89335000	-1.87336700	0.49037700

O	0.20122100	2.65530700	2.71156600
O	0.91247100	0.27302700	-0.91768300

8.1.4. Optimized geometries of adiabatic S_1 exciton state in $(\text{TiO}_2)_n$ with $n=4, 8, 16, 35, 84$ in vacuum at CAM-B3LYP/6-31G(d) level.

$(\text{TiO}_2)_{4a}$

Ti	1.99578700	-0.03806500	0.66156100
Ti	-0.00364600	-1.31873300	-0.87455700
Ti	0.13714500	1.50185000	-0.84403800
Ti	-2.00836600	-0.05450900	0.61901500
O	2.75436900	-0.07185800	2.06176100
O	1.65415100	-1.63927600	-0.31129800
O	1.80142800	1.62201000	-0.36035600
O	-0.00674300	0.06869300	0.57917400
O	-0.07408700	0.05394700	-2.00964500
O	-1.90628300	1.55234300	-0.42828000
O	-1.63248400	-1.69737900	-0.26023800
O	-2.71102200	0.02084700	2.05204200

$(\text{TiO}_2)_{4b}$

Ti	-2.30450400	0.30255300	0.39630500
Ti	2.55964400	-0.05792200	-0.35562300
O	0.91112200	-0.75904700	0.60852600
O	-3.64778800	1.13491200	0.11929400
O	3.91844000	-0.85954900	-0.13667800
O	1.46653600	-0.42545500	-1.86368300
Ti	0.50201500	1.02034800	1.26600500
O	-1.75629700	-1.15957000	-0.70284100
Ti	-0.07746200	-0.58058600	-0.95411500
O	-1.40279400	0.54953300	2.04899300
O	-0.60463200	1.08044300	-0.36553300
O	2.07014400	1.51185700	0.75298000

$(\text{TiO}_2)_{4c}$

Ti	-1.62012200	0.00000000	0.83143900
Ti	1.62012200	0.00000000	0.83143900
O	0.00000000	0.00000000	1.75420400
O	-2.98159500	0.00000000	1.72254100
O	2.98159500	0.00000000	1.72254100
O	1.41432200	-1.45209200	-0.38538000
Ti	0.00000000	1.42642100	-1.40049200
O	0.00000000	0.00000000	-2.51966100
Ti	0.00000000	-1.42642100	-1.40049200
O	-1.41432200	-1.45209200	-0.38538000
O	-1.41432200	1.45209200	-0.38538000
O	1.41432200	1.45209200	-0.38538000

 $(\text{TiO}_2)_{4d}$

Ti	-1.15645500	1.73045800	-0.72941800
Ti	0.17732300	0.04284400	-2.61289300
O	-0.63814900	-1.82308600	0.75079500
O	-1.62661800	0.57612400	-2.04156900
O	0.45222100	-0.01234600	-4.18011200
O	0.91278000	-1.38572100	-1.61813600
Ti	-0.34424600	-0.20465000	1.81503600
O	0.34689900	1.79461300	-1.73519300
Ti	0.94088400	-1.84369700	0.07459600
O	-1.15445300	1.29986900	0.97561100
O	1.43550900	-0.52979200	1.06440900
O	-0.47896100	-0.36799400	3.39654500

 $(\text{TiO}_2)_{8a}$

Ti	-3.24567600	-0.07876200	0.02283600
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Ti	-0.93758000	1.30365600	-1.76968400
Ti	-0.93983000	1.32741500	1.79582500
Ti	0.74946600	2.65923700	0.00257100
Ti	0.92383100	-1.32903100	1.76522700
Ti	3.20842500	0.12502900	0.02439500
Ti	0.97093600	-1.30449400	-1.80075800
Ti	-0.80465100	-2.64452900	0.05187800
O	0.43803800	-1.15562200	-0.04600000
O	-2.60090300	0.96594400	-1.50586500
O	-4.82095500	-0.26368600	0.01955900
O	-0.35569700	1.10745500	0.00725000
O	-0.07340400	2.91223700	-1.61778800
O	-2.60729500	0.97771700	1.52332600
O	-0.06109100	2.93904700	1.60859900
O	2.27416000	1.84725400	0.01509100
O	-0.02459900	-0.00264000	2.57460900
O	2.60359300	-0.96001600	1.50851900
O	4.78009600	0.33100100	0.04008000
O	2.61365400	-0.87998300	-1.56636000
O	-0.02429600	-0.04812500	-2.59682800
O	-2.32062000	-1.79490000	0.01509700
O	0.08160200	-2.93861700	1.66208200
O	0.17277700	-3.09558600	-1.73365100

(TiO₂)_{8b}

Ti	-1.38124200	-1.26949000	0.57029800
Ti	2.06901600	0.96547900	0.74647600
Ti	1.33362200	-2.48627500	0.08369900
O	1.28919300	-0.55590700	-0.01397100
Ti	-0.02977400	1.37040500	-1.43363900

Ti	2.41394600	-0.53424900	-1.64941900
Ti	-3.24903500	0.34146600	-0.82891600
O	1.99056500	0.51477100	2.39734400
O	-3.31437500	0.55785300	-2.54689700
O	-0.42373900	-2.68145800	-0.13779700
O	-3.42165700	2.03900700	-0.55450000
O	-0.72456800	-0.93379300	2.14717000
O	-3.80663600	3.50951300	-3.21870800
O	1.80661600	-2.52379000	1.73813800
O	-3.13123000	-1.15853000	0.34971500
O	1.05473200	-1.49139000	4.43767600
Ti	-2.93198400	2.46430600	-2.39328300
O	0.93468800	2.09884300	-0.01931400
O	-1.29262800	0.21932800	-0.64711900
O	1.19884900	0.48825100	-2.49320700
Ti	1.03222200	-1.13619700	2.89138800
O	2.47633200	-2.32656900	-1.36824700
O	3.55076200	0.71401200	-0.48322500
O	-0.97093900	2.49926300	-2.30131000

(TiO₂)_{8c}

Ti	-2.25334400	-1.54789100	0.85464300
Ti	3.14645000	1.17159400	-0.07270900
Ti	1.08098400	0.41704500	1.66509900
O	-2.61976900	-0.76651400	2.44450200
Ti	-3.18326100	1.02090500	-0.66588600
Ti	2.10370900	-1.12773100	-2.02005100
Ti	-1.80791100	0.82924700	2.12359700
O	3.92463800	2.50593000	-0.44561700
O	-4.47956200	1.63456300	-1.34049300

O	1.88971400	-2.95218600	-1.07711400
O	-3.32157800	-0.92299200	-0.33290000
O	2.74264700	0.85839400	1.79692400
O	-2.77858300	1.80647200	1.08975900
O	-0.99287900	-0.12279800	0.67967200
O	-1.09390300	-2.98885400	0.63351200
O	-1.58565900	1.19444300	-1.75003500
Ti	-0.05912000	0.50560200	-1.35935700
O	-0.12756300	1.19941800	2.76455700
O	0.22285000	-1.40712800	-1.21496100
O	1.23178200	-1.47161000	1.47791900
Ti	0.57446000	-2.47781100	0.22562200
O	1.13340500	1.21602600	-0.06632800
O	3.42766000	-0.37212300	-1.18041500
O	1.13965000	0.30386100	-2.68080700

 $(\text{TiO}_2)_{8d}$

Ti	3.22419200	0.13887900	-0.76599900
Ti	-1.13100400	0.03406200	-2.59161900
Ti	-1.27959000	-2.51716000	1.69499800
Ti	0.70134600	1.97541600	-1.67847800
O	4.81078200	0.13015800	-0.76946600
O	-0.56697500	0.64701700	1.27522800
O	-0.18754000	-1.63781700	2.97022400
Ti	-2.26221200	0.20297500	0.41476400
Ti	0.87202800	-0.54236700	1.61905000
Ti	0.70560200	-1.63866300	-1.34956800
Ti	-1.01704900	2.57207400	1.18467000
O	2.41080400	1.67692100	-1.58666900
O	-2.45968300	0.09494000	-1.45201400

O	-0.73274800	3.43440900	2.49329800
O	-1.54303300	-4.08764600	1.85836200
O	-0.42301500	-1.63658500	-2.78129100
O	-0.00631600	2.93435800	-0.40700000
O	2.38004700	-1.42777700	-1.59982800
O	-2.76819500	1.78700500	0.91064600
O	2.41280400	-0.09694700	0.98636900
O	0.16498200	0.17380900	-1.19922500
O	-2.66058700	-1.31605100	1.22138300
O	0.16358000	-2.02775400	0.37424900
O	-0.41575600	1.58414800	-3.13293800

(TiO₂)_{16a}

Ti	3.31550000	-1.62905900	1.52387600
Ti	2.48695300	0.45432500	-2.68980000
Ti	-0.41593600	1.57464100	-2.45445600
Ti	1.68978400	0.44700800	3.35252000
Ti	1.86934400	2.52232400	1.55794300
Ti	1.51161700	-5.13614400	-2.13987000
Ti	0.45139500	-0.44477000	-0.02828200
Ti	-1.48828000	-1.18690700	-2.83584800
Ti	-1.15462000	-3.01813400	1.77446700
Ti	1.18860900	-2.52428800	-3.11617000
Ti	1.81982000	-3.79171200	0.39546900
Ti	-2.92729600	-1.70894200	-0.45653100
Ti	-3.48871900	1.17952500	1.50065000
Ti	3.86842800	0.95793800	-0.36821200
Ti	-1.28005300	-0.72798500	3.30477200
Ti	-0.95389600	2.95380000	-0.07216000

O	-2.56593700	-3.10842100	0.68792600
O	4.40489300	-0.46172900	0.56955600
O	0.18255100	-0.03012300	4.16275400
O	-3.60449800	-0.30428100	0.26529500
O	-2.55249100	0.38016600	2.99675100
O	0.50684200	3.50115700	0.94346200
O	-3.10296500	-1.80993300	-2.25239100
O	0.23029400	-6.06459400	-2.29873000
O	1.08223600	-3.32216800	-1.41782900
O	-2.41486600	2.62713400	0.77756300
O	-4.93059700	1.68646900	1.92847200
O	2.16752500	2.20941500	3.31393300
O	0.31944600	-3.99469100	1.41441000
O	1.81973800	-4.01911500	-3.69751400
O	-1.63500000	-2.52256700	3.43502300
O	2.29837000	-5.26197100	-0.40330400
O	3.40098800	-3.37286000	1.38969200
O	2.45208000	-1.16935100	-3.39547000
O	3.39598500	2.42790700	0.60200400
O	2.89706200	-0.84680600	3.14697500
O	4.13542200	1.05372900	-2.15586800
O	-0.52487600	-2.31112800	-3.80523100
O	-1.00787900	3.19122700	-1.89527700
O	2.20316700	0.41121100	-0.84436300
O	-1.12849400	-1.33233600	-0.85520700
O	-0.37373600	1.28880500	-0.55514600
O	1.80970400	-1.72421000	0.57487600
O	0.31548000	-0.56509300	-2.11013900
O	-0.63680200	-1.21265700	1.61819400
O	1.24030900	1.64703400	-3.22174700

O	-1.65403800	0.57834900	-3.29085500
O	1.23371800	0.77114800	1.57878400

(TiO₂)_{16b}

O	-0.17980000	-0.03844400	-0.13327000
Ti	-0.16071900	-0.06957600	1.80600000
O	1.75806900	0.10390500	2.11092300
O	0.44344700	-2.17526400	-2.22159200
Ti	0.90057100	-0.67203800	-1.32106900
O	-1.05595500	1.04339800	2.49695300
O	-0.43261500	-1.86281000	2.49404000
O	2.31945700	0.25947900	-2.01288900
O	4.45847500	-2.02532900	-1.85620500
Ti	3.66360500	-0.59442800	-1.14907800
O	2.25361500	-1.49567800	-0.25677200
O	0.33962200	-5.33637900	-1.93004400
O	0.20358800	-3.52636500	0.30751600
Ti	0.81529800	-3.72580500	-1.35277900
O	0.50922200	-4.89997800	2.89398900
O	4.01981200	-1.72158700	2.98835500
Ti	0.49914100	-3.24726000	2.05538000
O	2.29169700	-2.77365200	2.14223700
Ti	2.97799600	-0.95309300	1.58695200
O	4.19054100	-0.09441500	0.46923600
O	4.51878900	-3.46097700	0.65345700
Ti	4.18112800	-3.59448800	2.51156800
Ti	5.06867300	-6.27885000	2.49502200
O	3.30702900	-5.54652900	2.46039200
Ti	1.57486600	-6.19812600	2.31834000
O	5.56451000	-4.69131400	3.09430500

O	5.45306200	-7.85316400	3.31393500
Ti	4.92919900	-9.31190900	2.36928800
O	3.52004700	-10.21902900	3.10889700
O	1.40676900	-7.82973600	3.07960600
Ti	2.17156700	-9.30305500	2.32728900
O	3.55362000	-8.40821100	1.40397700
O	3.51701700	-7.06181200	-0.88885200
Ti	1.65496100	-6.40873400	-1.18954700
O	1.27916100	-6.40176500	0.56765500
O	1.41845400	-8.10509500	-1.56586700
O	1.60164800	-9.81499200	0.75938500
O	5.90079000	-9.95516500	1.09673100
O	3.86569700	-9.93809600	-1.13839900
Ti	2.71585900	-8.89256600	-0.46274600
O	6.15478000	-8.06158600	-1.42793100
O	5.71229000	-6.44012800	0.86424300
Ti	5.80570800	-9.86030400	-0.84381100
Ti	5.30240600	-6.65417300	-0.88037200
O	2.55497400	-4.37754000	-1.26714100
Ti	4.29055500	-3.68054500	-1.05625300
O	6.64745200	-10.97092400	-1.60395200
O	5.34936000	-4.98722400	-1.65171600

(TiO₂)_{16c}

Ti	-1.68925900	1.56947300	-2.32919500
Ti	-1.83389700	-1.55273400	-2.17542200
Ti	1.68929700	1.56949900	-2.32918900
Ti	1.83396900	-1.55270600	-2.17542900
Ti	-1.69353000	2.92728400	0.68913200
Ti	1.69353400	2.92730300	0.68914200

Ti	-1.71660600	-2.94022000	0.76108600
Ti	1.71664400	-2.94020000	0.76109900
Ti	-1.63789500	1.27804800	3.30216900
Ti	-1.62942700	-1.38687300	3.37831300
Ti	1.63789600	1.27806200	3.30218000
Ti	1.62945100	-1.38685900	3.37833100
Ti	1.37266500	4.50681300	-1.84038700
Ti	1.35840400	-4.41106100	-1.83849900
Ti	-1.37267100	4.50679200	-1.84039700
Ti	-1.35843100	-4.41113800	-1.83850200
O	2.26100200	-3.15898000	-2.85979000
O	2.16124300	3.27078000	-2.88786600
O	-2.26099400	-3.15905900	-2.85975400
O	-2.16122700	3.27074100	-2.88787800
O	-2.50931400	-2.62099000	2.35498900
O	-2.51816900	2.48301400	2.22135200
O	2.50934400	-2.62096700	2.35502300
O	2.51816500	2.48303900	2.22136800
O	1.99897300	-4.50052900	-0.12576300
O	-2.11957300	4.48995500	-0.20306800
O	2.11955700	4.48998300	-0.20305300
O	-1.99899000	-4.50057500	-0.12579200
O	-2.37294700	-0.02363100	4.34515700
O	2.37295300	-0.02360500	4.34517600
O	-2.49716000	0.01380500	-2.80710900
O	2.49721900	0.01386600	-2.80711300
O	0.00000800	-2.78892800	1.28609900
O	-0.00000100	2.93151000	1.28490900
O	0.00002500	-1.34412800	-2.48466400
O	0.00001800	1.25268100	-2.83154400

O	2.17296300	-1.64708400	-0.43408600
O	-1.89857100	1.63031400	-0.55014800
O	1.89860000	1.63034100	-0.55013700
O	-2.17294700	-1.64710600	-0.43409800
O	-0.00016700	-3.17163700	-1.33977000
O	0.00000200	3.41725800	-1.34660500
O	-0.00001100	5.61896300	-2.35357700
O	-0.00016500	-5.52579200	-2.40402200
O	-1.26563500	-0.07927900	2.20908600
O	1.26565500	-0.07926900	2.20909800
O	-0.00000500	1.75057300	3.92050600
O	0.00000600	-1.83674300	4.03307200

(TiO₂)_{16d}

Ti	3.06050800	0.86128300	1.33479900
Ti	-0.28942200	4.31478100	1.94898400
Ti	-1.07998600	0.47074700	4.53627000
Ti	1.60582500	1.65456600	3.64786300
Ti	0.02038500	-0.14277800	0.68453700
Ti	-2.35535000	-1.14767300	-1.82818000
Ti	2.71362200	-2.23065400	0.26206300
Ti	-1.92636300	1.97481800	1.87202500
Ti	2.12408400	-2.18264600	-3.17659300
Ti	0.40148300	-3.58578400	1.17133400
Ti	0.93598400	2.55694000	-0.39793900
Ti	-0.69118400	-4.12785700	-2.09827200
Ti	-1.91636500	-1.77655800	2.99062700
Ti	0.39289600	0.64749600	-2.59404800
Ti	-0.36558800	3.28941900	4.55436200
Ti	-3.39891200	-0.52251000	0.67726300

O	-1.70229300	-0.86135100	-0.03423200
O	1.35752000	0.47508700	1.86196000
O	-0.77088300	-3.05013400	2.56284800
O	3.64128600	-0.78205500	0.94172800
O	2.98442000	-2.34230000	-1.39259800
O	-3.99093700	-0.79627700	-0.95541200
O	0.65672800	-3.21738500	-2.89927200
O	0.66582200	2.47336700	-2.13169200
O	-1.92476700	-1.12465900	4.68445000
O	3.28325800	1.58887300	2.99748500
O	-2.14701400	-2.77502400	-2.16850300
O	-1.08903900	1.90771900	5.81661600
O	3.06515400	-2.69461400	-4.35945500
O	1.51666400	-0.28404600	-3.44278900
O	2.21189200	-3.76601400	1.14487800
O	0.68036800	4.17647300	0.38283400
O	-1.07256900	-5.50339200	-2.81412200
O	-1.31201700	0.02471500	-2.74010000
O	2.64790100	2.10052600	0.10930800
O	-0.34805700	-4.33736300	-0.13916900
O	1.37328900	2.90666700	4.92251700
O	-3.45090500	-1.73160000	2.03428800
O	-1.92054400	2.02204900	3.79502700
O	-0.65345300	1.67879800	0.50027500
O	-3.40009200	1.20485800	1.22641600
O	-1.96509700	3.73855600	1.62278500
O	-0.32117400	4.98124100	3.57816600
O	0.67395400	0.28642300	4.46019000
O	-1.21444700	-0.11858600	2.44606300
O	0.82064600	-1.86300000	0.52158300

O	0.23517700	2.69236000	2.70809200
O	0.87530300	0.30238100	-0.82099000

8.2. Optimized geometries of neutral, cationic and anionic $(\text{TiO}_2)_n$ with $n = 4, 8, 16, 35, 84$ in vacuum at B3LYP/6-31G(d) level.

8.2.1. Optimized geometries of neutral $(\text{TiO}_2)_n$ with $n = 4, 8, 16, 35, 84$ in vacuum at B3LYP/6-31G(d) level.

$(\text{TiO}_2)_{4a}$

Ti	2.02276400	-0.00004000	0.61476300
Ti	-0.00001200	-1.40686400	-0.87412800
Ti	-0.00006400	1.40707800	-0.87378100
Ti	-2.02265500	-0.00011600	0.61501400
O	2.75693200	-0.00020200	2.04199500
O	1.66761600	-1.68603900	-0.29118600
O	1.66755600	1.68616600	-0.29077400
O	0.00004800	-0.00006400	0.51903200
O	-0.00010900	0.00025100	-2.03658400
O	-1.66762300	1.68610400	-0.29056800
O	-1.66755700	-1.68610100	-0.29097900
O	-2.75664700	-0.00030300	2.04233700

$(\text{TiO}_2)_{4b}$

Ti	-2.28708800	0.28487700	0.47150400
Ti	2.55940600	0.00846700	-0.33617900
O	0.84669500	-0.77737800	0.55360900
O	-3.63142000	1.11276000	0.18326400
O	3.90418700	-0.81883600	-0.04840200
O	1.48383900	-0.42221800	-1.90227800
Ti	0.36851800	0.91848600	1.19843600
O	-1.77650000	-1.17241800	-0.71994800
Ti	-0.09607500	-0.62639200	-1.06226900
O	-1.21178600	0.71513300	2.03793900
O	-0.57391900	1.06967700	-0.41765400

O	2.04856800	1.46535800	0.85560900
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(TiO₂)_{4c}

Ti	-1.60013400	0.00000000	0.88096900
Ti	1.60013400	0.00000000	0.88096900
O	0.00000000	0.00000000	1.78507600
O	-2.93242800	0.00000000	1.79334400
O	2.93242800	0.00000000	1.79334400
O	1.37648600	-1.48700700	-0.44948700
Ti	0.00000000	1.56107800	-1.46034600
O	0.00000000	0.00000000	-2.41506300
Ti	0.00000000	-1.56107800	-1.46034600
O	-1.37648600	-1.48700700	-0.44948700
O	-1.37648600	1.48700700	-0.44948700
O	1.37648600	1.48700700	-0.44948700

(TiO₂)_{4d}

Ti	-1.15762300	1.76597500	-0.86699500
Ti	0.16353900	0.04611100	-2.52427800
O	-0.63673900	-1.83417700	0.71473600
O	-1.64168600	0.41538000	-1.84203500
O	0.33885400	0.15154600	-4.12297200
O	0.96482700	-1.45733200	-1.64698100
Ti	-0.35241900	-0.16667600	1.71755800
O	0.44792800	1.71347800	-1.52125700
Ti	0.96873600	-1.88654300	0.06027200
O	-1.15396100	1.33660700	0.84021800
O	1.45275800	-0.53579400	1.03511400
O	-0.52747900	-0.27195200	3.31629000

$(\text{TiO}_2)_{8a}$

Ti	-3.22130700	-0.13036300	0.00002900
Ti	-0.92805000	1.33659400	-1.79375000
Ti	-0.92801300	1.33648500	1.79384900
Ti	0.76513200	2.70061800	0.00007400
Ti	0.92804800	-1.33659400	1.79375100
Ti	3.22130600	0.13036300	-0.00002800
Ti	0.92801100	-1.33648500	-1.79384900
Ti	-0.76513300	-2.70061700	-0.00007300
O	0.33937200	-1.14078300	-0.00003700
O	-2.59846900	0.94589300	-1.51340100
O	-4.81070400	-0.32194800	0.00003900
O	-0.33937300	1.14078300	0.00003800
O	-0.06060900	2.96730100	-1.62474900
O	-2.59843800	0.94579800	1.51351300
O	-0.06057600	2.96720300	1.62492900
O	2.30034400	1.87205100	0.00003500
O	0.00002700	-0.00007700	2.60539400
O	2.59846800	-0.94589300	1.51340200
O	4.81070200	0.32194700	-0.00003800
O	2.59843600	-0.94579800	-1.51351200
O	-0.00002900	0.00007700	-2.60539400
O	-2.30034600	-1.87205100	-0.00003400
O	0.06060700	-2.96730100	1.62475000
O	0.06057500	-2.96720300	-1.62492800

 $(\text{TiO}_2)_{8b}$

Ti	-1.40500700	-1.28170000	0.58136800
Ti	2.11955100	1.00563100	0.74865500

Ti	1.34017600	-2.48778000	0.06654300
O	1.27155400	-0.53383600	-0.06171300
Ti	-0.01565200	1.35968800	-1.42512300
Ti	2.48220200	-0.46910700	-1.57839700
Ti	-3.27741600	0.34292500	-0.82457500
O	2.02146900	0.49726700	2.40253800
O	-3.34749800	0.55335300	-2.55695600
O	-0.42454200	-2.69771300	-0.13803600
O	-3.44133800	2.05659800	-0.55441100
O	-0.72850700	-0.93795400	2.16142900
O	-3.80277900	3.52546300	-3.24508100
O	1.81852800	-2.52160700	1.72532500
O	-3.16793800	-1.16563100	0.36711400
O	1.07488500	-1.49361300	4.46246300
Ti	-2.93381100	2.46554100	-2.40392700
O	0.91235100	2.11145900	-0.01190600
O	-1.31189700	0.20645700	-0.64725000
O	1.25434100	0.46395400	-2.48934500
Ti	1.04663100	-1.12898600	2.90254500
O	2.49294300	-2.26987900	-1.40125300
O	3.45618800	0.59548500	-0.49339500
O	-0.96169900	2.48883400	-2.31425700

(TiO₂)_{8c}

Ti	-2.19418600	-1.54459900	0.84137400
Ti	3.10370800	1.19948900	-0.06238000
Ti	0.98737200	0.39825800	1.62395300
O	-2.64137600	-0.83245200	2.46905400
Ti	-3.14261000	1.03458500	-0.63513700
Ti	2.02501600	-1.31666500	-1.98094200

Ti	-1.86626000	0.80844400	2.21431100
O	4.00120000	2.48169000	-0.42563600
O	-4.45976800	1.63747700	-1.31543400
O	1.92430700	-2.96450000	-1.10774100
O	-3.28356000	-0.92290700	-0.34752600
O	2.67864700	0.87486900	1.76323300
O	-2.84139300	1.79848000	1.16809300
O	-1.01968200	-0.04863300	0.75629600
O	-1.04089400	-2.99227700	0.50674700
O	-1.57640500	1.22369100	-1.79440600
Ti	0.03693900	0.64421300	-1.51950300
O	-0.13221500	1.16493500	2.81874100
O	0.36597000	-1.15179200	-1.00711100
O	1.20746000	-1.49363400	1.54560500
Ti	0.67815800	-2.52588500	0.20836100
O	1.11595000	1.35446200	-0.15373600
O	3.24596400	-0.44200400	-1.14757300
O	1.14247700	0.12061700	-2.86950900

(TiO₂)_{8d}

Ti	3.23098400	0.09965800	-0.67803800
Ti	-1.12478000	0.07852200	-2.58494400
Ti	-1.23345600	-2.54106400	1.79114600
Ti	0.75408700	2.00227700	-1.66926400
O	4.83048000	0.08568600	-0.62611400
O	-0.63785500	0.68076500	1.18306400
O	0.16866700	-1.61671200	2.78026000
Ti	-2.37892900	0.19699600	0.48785200
Ti	0.71318000	-0.61861700	1.44499900
Ti	0.72775900	-1.67050100	-1.47841000

Ti	-1.09551000	2.62048800	1.13309600
O	2.46705500	1.68005700	-1.51524400
O	-2.43957200	0.08272700	-1.39429200
O	-0.79085900	3.46395800	2.46326600
O	-1.56368600	-4.08498100	2.07991600
O	-0.41088600	-1.58357600	-2.90935400
O	0.00003700	2.97194700	-0.42104900
O	2.41727200	-1.45082200	-1.64773300
O	-2.86351100	1.81920300	0.95038200
O	2.36650800	-0.18302900	1.03929700
O	0.24325100	0.15582100	-1.23697400
O	-2.64883600	-1.32955900	1.36759300
O	0.07100600	-2.03741800	0.25102000
O	-0.40994100	1.63557800	-3.12132900

(TiO₂)_{16a}

Ti	3.26329100	-1.57660400	1.45609300
Ti	2.35247600	0.35995400	-2.68600700
Ti	-0.34313200	1.54522600	-2.41701500
Ti	1.69582400	0.47112500	3.38078800
Ti	1.89941800	2.55840400	1.58069600
Ti	1.54558500	-5.24077400	-2.19811000
Ti	0.41258900	-0.43811500	-0.09418000
Ti	-1.38105500	-1.22455400	-2.72012600
Ti	-1.18242600	-2.97720700	1.77675000
Ti	1.33019900	-2.60303300	-3.21463500
Ti	1.78262300	-3.84901900	0.32527700
Ti	-2.98233500	-1.73849600	-0.43963400
Ti	-3.52958100	1.19674100	1.50519800

Ti	3.85328400	1.02024300	-0.41053200
Ti	-1.28685400	-0.67828900	3.33593900
Ti	-0.96743700	2.97873100	-0.01438300
O	-2.65128900	-3.11880600	0.75774100
O	4.37870700	-0.45308000	0.52956100
O	0.17911600	0.02118300	4.21525600
O	-3.63683800	-0.29097600	0.25932000
O	-2.58173400	0.42378000	3.02240300
O	0.50496900	3.53664100	0.98908900
O	-3.04794400	-1.85465400	-2.26216800
O	0.20955100	-6.10664600	-2.38302500
O	1.18108000	-3.38270800	-1.49006800
O	-2.46728300	2.68155800	0.80446700
O	-4.99302200	1.68766000	1.93495200
O	2.21823300	2.22822000	3.35005800
O	0.27991900	-3.98011100	1.37640000
O	1.91346600	-4.14819500	-3.77172100
O	-1.62755800	-2.48901500	3.46228600
O	2.22757100	-5.38016200	-0.39527200
O	3.36360900	-3.33193900	1.26928300
O	2.54972600	-1.23278700	-3.50578100
O	3.42345900	2.50723700	0.60747300
O	2.87551400	-0.87735400	3.11415700
O	4.05229800	1.01880400	-2.19383100
O	-0.41432200	-2.31067700	-3.76322500
O	-0.95189900	3.18427800	-1.83605700
O	2.15769800	0.52295900	-0.75702300
O	-1.16653100	-1.39398400	-0.76399200
O	-0.42037900	1.24984600	-0.42968000
O	1.69519200	-1.67161700	0.48100600

O	0.50236900	-0.45932700	-2.06864200
O	-0.64445200	-1.14876500	1.63375400
O	1.25588600	1.67815200	-3.30050300
O	-1.59564900	0.54563900	-3.21474700
O	1.22434900	0.80185000	1.61737900

(TiO₂)_{16b}

O	-0.03154200	0.04738000	-0.01324000
Ti	-0.01131400	0.00610000	1.94841600
O	1.86055800	0.01209900	2.51613600
O	0.04938400	-2.10163900	-2.28466100
Ti	0.72343900	-0.60329000	-1.43807800
O	-0.91604600	1.14005300	2.63011700
O	-0.46762200	-1.80369200	2.47802900
O	2.25180200	0.24515700	-2.03183900
O	4.44472300	-2.15809400	-1.91962200
Ti	3.45730900	-0.81981400	-1.17239200
O	1.97668100	-1.81615000	-0.67688400
O	0.34314400	-5.18288100	-1.99431000
O	0.00230000	-3.52765300	0.21307900
Ti	0.77358300	-3.51056800	-1.38328100
O	0.39348000	-4.81978600	2.85573500
O	4.32523100	-1.96663200	3.02253300
Ti	0.41811000	-3.19950200	1.95001000
O	2.23415800	-2.78609200	1.93258500
Ti	3.09394100	-1.07439000	1.97431500
O	3.93236900	-0.36104900	0.48238700
O	4.57661600	-3.57876100	0.64816200
Ti	4.17257600	-3.66902400	2.40672100
Ti	5.01122600	-6.41073900	2.53183300

O	3.19644900	-5.48293600	2.48783700
Ti	1.47201600	-6.12181900	2.28034500
O	5.44167100	-4.73842700	3.14285600
O	5.73541300	-7.81966800	3.43322200
Ti	5.06136400	-9.31801700	2.58663900
O	3.53300100	-10.16646300	3.18040100
O	1.34008300	-7.76320700	3.06817500
Ti	2.32749400	-9.10149600	2.32095200
O	3.80812200	-8.10516300	1.82543300
O	3.55065700	-7.13520300	-0.78402800
Ti	1.61223800	-6.25228200	-1.25817200
O	1.20819400	-6.34254100	0.50038800
O	1.45958700	-7.95468000	-1.87397000
O	1.85243300	-9.56026600	0.66617600
O	5.81635600	-9.96868700	1.16180500
O	3.92425100	-9.93340300	-1.36756400
Ti	2.69087400	-8.84691000	-0.82574100
O	6.25243000	-8.11761700	-1.32947500
O	5.78251900	-6.39366700	0.93547800
Ti	5.79612500	-9.92740600	-0.79985000
Ti	5.36670600	-6.72180200	-0.80145500
O	2.58836500	-4.43837000	-1.33928900
Ti	4.31279500	-3.79948600	-1.13179600
O	6.70085200	-11.06136200	-1.48155500
O	5.39133700	-5.10151600	-1.70718000

(TiO₂)_{16c}

Ti	-1.72196900	1.58204700	-2.28319600
Ti	-1.72196900	-1.58204700	-2.28319600
Ti	1.72196900	1.58204700	-2.28319600

Ti	1.72196900	-1.58204700	-2.28319600
Ti	-1.70715100	3.01369200	0.73019100
Ti	1.70715100	3.01369200	0.73019100
Ti	-1.70715100	-3.01369200	0.73019100
Ti	1.70715100	-3.01369200	0.73019100
Ti	-1.64859800	1.34137500	3.34296700
Ti	-1.64859800	-1.34137500	3.34296700
Ti	1.64859800	1.34137500	3.34296700
Ti	1.64859800	-1.34137500	3.34296700
Ti	1.38035800	4.55944900	-1.83042300
Ti	1.38035800	-4.55944900	-1.83042300
Ti	-1.38035800	4.55944900	-1.83042300
Ti	-1.38035800	-4.55944900	-1.83042300
O	2.17167900	-3.29716200	-2.86907000
O	2.17167900	3.29716200	-2.86907000
O	-2.17167900	-3.29716200	-2.86907000
O	-2.17167900	3.29716200	-2.86907000
O	-2.53442200	-2.57161200	2.28547600
O	-2.53442200	2.57161200	2.28547600
O	2.53442200	-2.57161200	2.28547600
O	2.53442200	2.57161200	2.28547600
O	2.14612000	-4.57415300	-0.18031600
O	-2.14612000	4.57415300	-0.18031600
O	2.14612000	4.57415300	-0.18031600
O	-2.14612000	-4.57415300	-0.18031600
O	-2.39868500	0.00000000	4.35506200
O	2.39868500	0.00000000	4.35506200
O	-2.49717100	0.00000000	-2.78952300
O	2.49717100	0.00000000	-2.78952300
O	0.00000000	-3.01984400	1.33268900

O	0.00000000	3.01984400	1.33268900
O	0.00000000	-1.32563300	-2.72953300
O	0.00000000	1.32563300	-2.72953300
O	1.94542700	-1.69266800	-0.49362700
O	-1.94542700	1.69266800	-0.49362700
O	1.94542700	1.69266800	-0.49362700
O	-1.94542700	-1.69266800	-0.49362700
O	0.00000000	-3.49626500	-1.28324000
O	0.00000000	3.49626500	-1.28324000
O	0.00000000	5.66876400	-2.38179000
O	0.00000000	-5.66876400	-2.38179000
O	-1.27579900	0.00000000	2.20343300
O	1.27579900	0.00000000	2.20343300
O	0.00000000	1.80084200	3.98111200
O	0.00000000	-1.80084200	3.98111200

(TiO₂)_{16d}

Ti	3.07373000	0.82760300	1.32175800
Ti	-0.34357800	4.32550200	1.98923900
Ti	-1.21525500	0.67655700	4.99951300
Ti	1.59098200	1.56943300	3.60397000
Ti	0.01520400	-0.19752400	0.57853800
Ti	-2.39783100	-1.14322800	-1.96924100
Ti	2.78528700	-2.30344300	0.24542700
Ti	-1.90029500	1.88933800	1.85190400
Ti	2.10704600	-2.18381300	-3.18954900
Ti	0.41255300	-3.56507600	1.22610600
Ti	0.94325100	2.56359800	-0.41862700
Ti	-0.75935900	-4.09558200	-2.06404700
Ti	-1.87610800	-1.70678700	3.06556200

Ti	0.38268400	0.68603000	-2.67956900
Ti	-0.33315900	3.28634500	4.64458300
Ti	-3.19036300	-0.59119300	0.69319500
O	-1.57056000	-0.98112000	-0.26369600
O	1.35529800	0.48161600	1.85034600
O	-0.67554400	-2.98145500	2.67916500
O	3.67807200	-0.81787700	0.92907200
O	3.03903600	-2.38197500	-1.42908600
O	-3.93274200	-0.80978700	-0.91397500
O	0.62614400	-3.18965800	-2.83184400
O	0.68361700	2.53426600	-2.15957400
O	-2.04389500	-0.97498000	4.72933500
O	3.30932700	1.47773700	3.02507300
O	-2.23629600	-2.78463000	-2.35831400
O	-0.97994600	2.14994900	6.04082400
O	2.99439000	-2.74686900	-4.41022700
O	1.51282400	-0.27522100	-3.51777600
O	2.22867700	-3.83081400	1.14326400
O	0.63600000	4.19939600	0.46820000
O	-1.05427900	-5.52847000	-2.73935500
O	-1.32949300	0.07652200	-2.85708000
O	2.65927600	2.11931700	0.10728500
O	-0.43459000	-4.25864000	-0.07647200
O	1.40438400	2.91465400	4.86265700
O	-3.38418200	-1.81665300	2.03611500
O	-1.84004500	1.89869500	3.77481200
O	-0.63416600	1.68843800	0.44818800
O	-3.39196700	1.17946600	1.20107000
O	-1.95937600	3.73254500	1.62151200
O	-0.51110700	4.88419400	3.79543200

O	0.49658200	0.38879700	4.48289600
O	-1.33301000	-0.19797900	2.09122400
O	0.91668600	-1.86066000	0.52847800
O	0.21728500	2.71166300	2.75804800
O	0.89652300	0.32765400	-0.91009100

(TiO₂)_{35,G09-opt}

O	11.40598700	14.73460300	30.23151700
O	6.25719200	14.73669200	30.10563500
O	10.47300100	13.18184300	28.38158200
O	10.50746900	13.15579800	32.59976000
O	10.73397500	11.42843500	30.21967200
O	8.75652300	13.65956600	30.87078300
O	6.99873300	13.12293800	28.26344700
O	6.93378600	13.10724500	32.51484700
O	8.67126200	15.26263700	33.52317000
O	6.76875600	11.38721800	30.14144300
O	10.78333700	15.26001400	26.57288800
O	12.24093500	17.06593900	21.88230200
O	10.93144500	16.77828700	19.13322000
O	12.04446800	14.94736300	23.90262900
O	12.92345700	14.63304100	27.70784500
O	10.69722500	17.49728200	24.01356100
O	13.20414900	16.50975500	25.34886800
O	10.48517900	15.04541900	20.84741000
O	6.79216900	14.83646900	26.00415200
O	8.98859100	17.27776600	21.71162400
O	7.16092100	17.05165500	19.37697300
O	9.32555100	15.05654900	23.83252800

O	8.34849600	15.44806700	27.96470700
O	7.11050800	16.54211600	23.28788900
O	8.57588900	16.83186000	25.57018800
O	6.77789100	15.08842400	20.80341900
O	5.43373600	17.47137700	21.77307000
O	4.68067000	14.95948500	23.68070200
O	4.87138100	15.19276000	27.64100600
O	4.98102600	16.88247700	25.22546600
O	10.68312100	11.40364000	26.17800000
O	12.48194400	13.50989800	21.58992900
O	10.99630900	13.16822100	19.12612100
O	13.17769900	11.38285400	23.10505400
O	12.41873800	11.05446300	27.93078700
O	10.68028200	12.73630600	23.16494800
O	12.90015700	13.03038700	25.37148300
O	10.88067600	11.26597600	20.80309900
O	6.92096200	11.14463200	26.23790300
O	8.81436600	13.15703700	21.56598000
O	6.62984500	12.96752200	19.24718000
O	8.50809000	11.31928000	23.91848000
O	8.81498300	10.91722100	27.92301400
O	7.01903100	13.54434300	23.24839300
O	8.84893200	13.21484100	25.52301500
O	7.07416800	11.18190500	21.09635400
O	5.10561700	12.97938800	21.67874400
O	5.57144600	11.31137900	23.83519500
O	5.04541400	11.15595500	27.79778500
O	4.64035800	13.07213500	25.42812700
O	12.34371800	8.82260200	21.75879200
O	10.81008300	9.38586400	19.25560400

O	10.73264700	9.91495000	23.27266700
O	12.86274700	9.77724600	25.21943100
O	8.94047300	9.03837600	21.64130100
O	6.77428100	9.31800400	19.44618800
O	7.10826000	8.94895800	23.41456400
O	9.02053800	9.39925900	25.42150600
O	5.15824000	9.24611400	21.88334400
O	4.52487700	9.63475000	25.30918200
O	10.44285200	15.12561400	16.84512000
O	7.00491200	15.52317600	16.99330700
O	8.60933300	14.89037700	14.55707700
O	8.76551300	14.81328100	18.70790200
O	10.50819600	11.09057200	16.92253700
O	7.09028800	10.75619200	17.07415400
O	6.53791300	13.01546400	13.70246700
O	8.70870200	11.27453200	14.60642800
O	8.82847300	11.35056200	18.84740500
O	8.28589300	13.09825800	16.26593700
Ti	11.32779700	14.76191100	28.42495700
Ti	6.56080800	14.88362300	28.35787500
Ti	10.56034400	13.18831800	30.85400100
Ti	10.64184300	11.38230500	28.43666700
Ti	6.95840400	13.12619500	30.76898900
Ti	8.70249700	13.77621600	32.93135000
Ti	6.79420400	11.36560900	28.32855600
Ti	12.51651300	14.93325600	25.87491500
Ti	10.69021200	16.78795800	20.91580800
Ti	12.23493200	16.74888600	23.69649400
Ti	10.56687200	15.00404700	18.61758700
Ti	8.73804200	15.15670800	26.24090900

Ti	7.05318900	16.86721000	21.21954500
Ti	8.95892800	16.75053400	23.79869200
Ti	7.07459700	15.35228100	18.78344000
Ti	5.07089400	15.03867600	25.86204000
Ti	5.31495300	16.64573100	23.49564400
Ti	12.45648200	11.28606000	26.14587500
Ti	10.70171600	13.13893800	21.07017900
Ti	12.40562200	13.09125300	23.30508500
Ti	10.59200000	11.13423400	18.73066600
Ti	8.79344800	11.14991800	25.98075000
Ti	6.88819100	13.13002700	21.06268300
Ti	8.84610300	13.21506400	23.63419900
Ti	7.05075100	11.06876900	18.82229800
Ti	5.09085100	11.25897400	25.96909000
Ti	5.29885900	13.15041200	23.43239700
Ti	10.75071500	9.44416900	21.08714700
Ti	12.51499900	9.78378400	23.37308100
Ti	6.93485000	9.42996900	21.22092700
Ti	8.89390300	9.60778600	23.63795000
Ti	5.40324000	9.54705500	23.64546200
Ti	8.64295100	14.91496900	16.30378500
Ti	8.74724600	11.29564300	16.35010100
Ti	8.04983900	13.06273100	14.21994800

(TiO₂)₃₅,FHI-Aims

Ti	17.21728000	17.00418000	43.79675000
Ti	17.05413000	15.25427000	46.13111000
Ti	20.77919000	17.00424000	43.79676000
Ti	18.99823000	17.20380000	41.34950000
Ti	20.94236000	15.25433000	46.13106000

Ti	17.21729000	20.98931000	43.79685000
Ti	16.99297000	18.99667000	46.12812000
Ti	18.99748000	18.99682000	38.84041000
Ti	20.77917000	20.98927000	43.79686000
Ti	18.99823000	20.78978000	41.34956000
Ti	21.00353000	18.99672000	46.12814000
Ti	17.05414000	22.73905000	46.13130000
Ti	20.94237000	22.73915000	46.13126000
Ti	15.36054000	15.35862000	48.51730000
Ti	17.00577000	17.21550000	53.23768000
Ti	15.25579000	17.05240000	50.90335000
Ti	18.99823000	15.31850000	48.63359000
Ti	20.99081000	17.21550000	53.23767000
Ti	18.99825000	16.99120000	50.90635000
Ti	22.63593000	15.35878000	48.51723000
Ti	22.74068000	17.05244000	50.90330000
Ti	15.32030000	18.99653000	48.40089000
Ti	17.00572000	20.77742000	53.23779000
Ti	15.25586000	20.94060000	50.90342000
Ti	17.20530000	18.99640000	55.68493000
Ti	18.99827000	18.99654000	48.51726000
Ti	20.99085000	20.77745000	53.23777000
Ti	18.99828000	21.00177000	50.90646000
Ti	20.79134000	18.99641000	55.68488000
Ti	22.67625000	18.99665000	48.40085000
Ti	22.74073000	20.94065000	50.90337000
Ti	15.36050000	22.63427000	48.51737000
Ti	18.99832000	22.67452000	48.63377000
Ti	22.63618000	22.63440000	48.51730000
Ti	18.99833000	18.99709000	58.19391000

O	18.99530000	18.99685000	37.22212000
O	17.07568000	17.06219000	46.00766000
O	17.13241000	15.04662000	48.38093000
O	16.94454000	15.23026000	44.30900000
O	17.27025000	16.81318000	41.99497000
O	15.30522000	14.83963000	46.71770000
O	20.92086000	17.06225000	46.00763000
O	18.99823000	17.20814000	43.91761000
O	20.86404000	15.04677000	48.38088000
O	21.05196000	15.23030000	44.30893000
O	18.99823000	17.23104000	39.55068000
O	20.72625000	16.81344000	41.99495000
O	18.99826000	14.84362000	46.58883000
O	22.69129000	14.83925000	46.71758000
O	17.07556000	20.93111000	46.00770000
O	17.09066000	18.99674000	48.24686000
O	16.79070000	18.99670000	44.20579000
O	17.27027000	21.18037000	41.99507000
O	15.17775000	18.99655000	46.59378000
O	18.99785000	18.99679000	41.51076000
O	20.92096000	20.93118000	46.00769000
O	18.99823000	20.78528000	43.91776000
O	20.90588000	18.99678000	48.24688000
O	21.20577000	18.99672000	44.20580000
O	18.99822000	20.76259000	39.55074000
O	20.72622000	21.18012000	41.99505000
O	18.99827000	18.99666000	46.57202000
O	22.81876000	18.99660000	46.59374000
O	17.13243000	22.94595000	48.38106000
O	16.94460000	22.76320000	44.30917000

O	15.30526000	23.15435000	46.71779000
O	20.86422000	22.94575000	48.38101000
O	21.05184000	22.76318000	44.30911000
O	18.99827000	23.14981000	46.58913000
O	22.69118000	23.15390000	46.71782000
O	14.84098000	15.30363000	50.31676000
O	16.81499000	17.26835000	55.03950000
O	15.23184000	16.94288000	52.72550000
O	15.04946000	17.13059000	48.65363000
O	17.06377000	17.07381000	51.02686000
O	18.99828000	15.17602000	50.44072000
O	21.18158000	17.26836000	55.03947000
O	18.99829000	16.78894000	52.82867000
O	18.99821000	17.08889000	48.78754000
O	20.93272000	17.07384000	51.02685000
O	23.15593000	15.30361000	50.31677000
O	22.76474000	16.94286000	52.72545000
O	22.94728000	17.13074000	48.65357000
O	14.84510000	18.99648000	50.44552000
O	16.81471000	20.72444000	55.03956000
O	15.23179000	21.05010000	52.72554000
O	17.23250000	18.99636000	57.48374000
O	17.20972000	18.99647000	53.11699000
O	15.04879000	20.86238000	48.65365000
O	17.06381000	20.91911000	51.02693000
O	18.99827000	18.99648000	50.46249000
O	21.18183000	20.72446000	55.03952000
O	18.99828000	21.20400000	52.82879000
O	20.76414000	18.99637000	57.48369000
O	20.78684000	18.99648000	53.11695000

O	18.99823000	20.90417000	48.78773000
O	20.93277000	20.91909000	51.02689000
O	18.99832000	18.99680000	55.52376000
O	23.15142000	18.99654000	50.44550000
O	22.76477000	21.05013000	52.72548000
O	22.94787000	20.86250000	48.65358000
O	14.84081000	22.68951000	50.31697000
O	18.99830000	22.81701000	50.44089000
O	23.15519000	22.68954000	50.31682000
O	18.99834000	18.99928000	59.81226000

(TiO₂)₈₄,FHI-Aims

Ti	17.22287000	17.07534000	43.83230000
Ti	17.06650000	15.34986000	46.19808000
Ti	20.77379000	17.07554000	43.83243000
Ti	18.99842000	17.20064000	41.35711000
Ti	20.93026000	15.34987000	46.19803000
Ti	17.22287000	20.91795000	43.83235000
Ti	16.85775000	18.99661000	46.26068000
Ti	18.99666000	18.99670000	38.87121000
Ti	20.77377000	20.91776000	43.83249000
Ti	18.99841000	20.79269000	41.35712000
Ti	21.13897000	18.99662000	46.26086000
Ti	17.06647000	22.64338000	46.19815000
Ti	20.93024000	22.64338000	46.19810000
Ti	13.54957000	13.54673000	53.36872000
Ti	17.20496000	13.42554000	53.44122000
Ti	15.16232000	13.40503000	50.92749000
Ti	20.79183000	13.42567000	53.44116000

Ti	18.99837000	13.32249000	50.93801000
Ti	24.44748000	13.54700000	53.36836000
Ti	22.83444000	13.40496000	50.92742000
Ti	13.42798000	17.20326000	53.29550000
Ti	13.40669000	15.16051000	55.80911000
Ti	15.34876000	15.12403000	48.55860000
Ti	17.16408000	17.16213000	53.36829000
Ti	15.06463000	17.12888000	50.97909000
Ti	17.13065000	15.06264000	55.75744000
Ti	18.99840000	14.96653000	48.63895000
Ti	20.83280000	17.16213000	53.36824000
Ti	18.99840000	17.14621000	50.93509000
Ti	20.86615000	15.06267000	55.75740000
Ti	22.64801000	15.12403000	48.55855000
Ti	24.56901000	17.20325000	53.29537000
Ti	22.93219000	17.12886000	50.97904000
Ti	24.59005000	15.16052000	55.80901000
Ti	13.42796000	20.78985000	53.29552000
Ti	13.32412000	18.99653000	55.79856000
Ti	15.26960000	18.99660000	48.60111000
Ti	17.16407000	20.83098000	53.36833000
Ti	15.06463000	20.86428000	50.97913000
Ti	17.14806000	18.99653000	55.80136000
Ti	18.99833000	18.99660000	48.53254000
Ti	20.83279000	20.83098000	53.36828000
Ti	18.99838000	20.84696000	50.93513000
Ti	20.84875000	18.99653000	55.80134000
Ti	22.72712000	18.99662000	48.60119000
Ti	24.56901000	20.78994000	53.29539000
Ti	22.93217000	20.86434000	50.97907000

Ti	24.67263000	18.99656000	55.79845000
Ti	13.54951000	24.44633000	53.36878000
Ti	13.40668000	22.83255000	55.80919000
Ti	15.34873000	22.86916000	48.55867000
Ti	17.20495000	24.56755000	53.44131000
Ti	15.16229000	24.58813000	50.92759000
Ti	17.13063000	22.93042000	55.75752000
Ti	18.99837000	23.02666000	48.63903000
Ti	20.79181000	24.56743000	53.44124000
Ti	18.99834000	24.67069000	50.93811000
Ti	20.86613000	22.93041000	55.75748000
Ti	22.64799000	22.86921000	48.55863000
Ti	24.44755000	24.44616000	53.36841000
Ti	22.83441000	24.58827000	50.92754000
Ti	24.59005000	22.83260000	55.80909000
Ti	15.12582000	15.34687000	58.17791000
Ti	17.07732000	17.22102000	62.90411000
Ti	15.35174000	17.06459000	60.53845000
Ti	18.99843000	15.26782000	58.13522000
Ti	20.91969000	17.22099000	62.90409000
Ti	18.99848000	16.85586000	60.47570000
Ti	22.87103000	15.34689000	58.17784000
Ti	22.64522000	17.06460000	60.53837000
Ti	14.96842000	18.99650000	58.09754000
Ti	17.07730000	20.77190000	62.90415000
Ti	15.35173000	20.92837000	60.53848000
Ti	17.20256000	18.99644000	65.37938000
Ti	18.99843000	18.99652000	58.20402000
Ti	20.91969000	20.77195000	62.90413000
Ti	18.99847000	21.13712000	60.47575000

Ti	20.79456000	18.99645000	65.37928000
Ti	23.02844000	18.99652000	58.09747000
Ti	22.64521000	20.92839000	60.53841000
Ti	15.12581000	22.64614000	58.17799000
Ti	18.99841000	22.72522000	58.13530000
Ti	22.87100000	22.64616000	58.17791000
Ti	18.99857000	18.99644000	67.86529000
O	18.98991000	18.99672000	37.25400000
O	17.11742000	17.13473000	46.06449000
O	17.13422000	15.24979000	48.40555000
O	16.96244000	15.30568000	44.37882000
O	17.28117000	16.83438000	42.03727000
O	15.30236000	15.01307000	46.73950000
O	20.87928000	17.13475000	46.06453000
O	18.99833000	17.32910000	43.96199000
O	20.86255000	15.24986000	48.40551000
O	21.03427000	15.30583000	44.37873000
O	18.99867000	17.21557000	39.56107000
O	20.71576000	16.83530000	42.03726000
O	18.99838000	14.88797000	46.65174000
O	22.69438000	15.01309000	46.73942000
O	17.11740000	20.85850000	46.06453000
O	17.03275000	18.99661000	48.34199000
O	16.68529000	18.99663000	44.27298000
O	17.28116000	21.15898000	42.03732000
O	15.09193000	18.99660000	46.76504000
O	18.99710000	18.99666000	41.47771000
O	20.87928000	20.85850000	46.06457000
O	18.99832000	20.66421000	43.96201000
O	20.96393000	18.99661000	48.34202000

O	21.31143000	18.99664000	44.27313000
O	18.99866000	20.77781000	39.56108000
O	20.71574000	21.15808000	42.03731000
O	18.99833000	18.99662000	46.72297000
O	22.90477000	18.99662000	46.76511000
O	17.13419000	22.74343000	48.40562000
O	16.96242000	22.68760000	44.37889000
O	15.30233000	22.98015000	46.73956000
O	20.86254000	22.74337000	48.40557000
O	21.03425000	22.68747000	44.37880000
O	18.99836000	23.10526000	46.65183000
O	22.69436000	22.98016000	46.73949000
O	12.99929000	13.44026000	55.15525000
O	13.44163000	12.99957000	51.58163000
O	17.20248000	13.26668000	55.25411000
O	15.32018000	13.23683000	53.21983000
O	15.04191000	13.36321000	49.10533000
O	17.07151000	13.00071000	51.35919000
O	20.79459000	13.26667000	55.25402000
O	18.99839000	12.89516000	52.96843000
O	18.99842000	13.18214000	49.10821000
O	20.92534000	13.00055000	51.35926000
O	24.99734000	13.44013000	55.15507000
O	22.67674000	13.23827000	53.21958000
O	22.95470000	13.36321000	49.10521000
O	24.55500000	12.99909000	51.58142000
O	13.00193000	17.06952000	55.37717000
O	13.36498000	15.04045000	57.63143000
O	13.24398000	15.31794000	53.51754000
O	13.26854000	17.19953000	51.48274000

O	15.20203000	15.21130000	50.78685000
O	17.09374000	17.07579000	55.33601000
O	15.20076000	17.24310000	53.07312000
O	17.06554000	14.90187000	57.73996000
O	17.24250000	15.19853000	53.66309000
O	14.90376000	17.06353000	48.99653000
O	17.07767000	17.09224000	51.40037000
O	15.21309000	15.19939000	55.95008000
O	18.99844000	15.10237000	50.71650000
O	20.90305000	17.07583000	55.33598000
O	18.99841000	17.15225000	52.98456000
O	20.93138000	14.90186000	57.73991000
O	20.75380000	15.19860000	53.66315000
O	18.99835000	17.07700000	49.04084000
O	20.91916000	17.09221000	51.40037000
O	18.99842000	15.21507000	56.14325000
O	22.79497000	15.21129000	50.78669000
O	24.99476000	17.06957000	55.37711000
O	22.79616000	17.24251000	53.07317000
O	24.63188000	15.04034000	57.63128000
O	24.75433000	15.31806000	53.51717000
O	23.09301000	17.06359000	48.99649000
O	24.72826000	17.19985000	51.48257000
O	22.78371000	15.19960000	55.94991000
O	13.00194000	20.92353000	55.37723000
O	13.18394000	18.99650000	57.62831000
O	12.89686000	18.99655000	53.76813000
O	13.26854000	20.79356000	51.48277000
O	15.21619000	18.99658000	50.59295000
O	17.09374000	20.91727000	55.33605000

O	15.20075000	20.75009000	53.07317000
O	17.07875000	18.99652000	57.69559000
O	17.15615000	18.99655000	53.75190000
O	14.90375000	20.92965000	48.99656000
O	17.07765000	20.90091000	51.40040000
O	15.10404000	18.99652000	56.01978000
O	18.99842000	18.99659000	50.66080000
O	20.90303000	20.91724000	55.33602000
O	18.99840000	20.84084000	52.98458000
O	20.91808000	18.99652000	57.69557000
O	20.84093000	18.99656000	53.75179000
O	18.99834000	20.91623000	49.04088000
O	20.91915000	20.90096000	51.40041000
O	18.99840000	18.99652000	56.07587000
O	22.78039000	18.99660000	50.59302000
O	24.99472000	20.92354000	55.37717000
O	22.79616000	20.75074000	53.07322000
O	24.81289000	18.99653000	57.62821000
O	25.09999000	18.99660000	53.76803000
O	23.09299000	20.92962000	48.99652000
O	24.72824000	20.79330000	51.48260000
O	22.89273000	18.99654000	56.01975000
O	12.99934000	24.55282000	55.15533000
O	13.36497000	22.95259000	57.63150000
O	13.24376000	22.67514000	53.51758000
O	13.44162000	24.99356000	51.58174000
O	15.20198000	22.78186000	50.78690000
O	17.20240000	24.72639000	55.25420000
O	15.32014000	24.75606000	53.21990000
O	17.06551000	23.09116000	57.74005000

O	17.24257000	22.79457000	53.66318000
O	15.04189000	24.62997000	49.10543000
O	17.07147000	24.99245000	51.35930000
O	15.21308000	22.79363000	55.95013000
O	18.99842000	22.89081000	50.71659000
O	20.79463000	24.72641000	55.25411000
O	18.99837000	25.09797000	52.96855000
O	20.93136000	23.09119000	57.73999000
O	20.75367000	22.79451000	53.66324000
O	18.99839000	24.81105000	49.10831000
O	20.92531000	24.99263000	51.35937000
O	18.99840000	22.77803000	56.14333000
O	22.79497000	22.78193000	50.78675000
O	24.99697000	24.55299000	55.15511000
O	22.67676000	24.75461000	53.21965000
O	24.63184000	22.95274000	57.63134000
O	24.75454000	22.67512000	53.51721000
O	22.95465000	24.63001000	49.10532000
O	24.55493000	24.99389000	51.58156000
O	22.78370000	22.79344000	55.94995000
O	15.01502000	15.30048000	59.99708000
O	16.83661000	17.27910000	64.69922000
O	15.30761000	16.96057000	62.35773000
O	15.25170000	17.13234000	58.33091000
O	17.13662000	17.11559000	60.67199000
O	18.99849000	15.09010000	59.97132000
O	21.16035000	17.27911000	64.69919000
O	18.99851000	16.68336000	62.46343000
O	18.99844000	17.03099000	58.39451000
O	20.86035000	17.11561000	60.67197000

O	22.98194000	15.30049000	59.99699000
O	22.68938000	16.96058000	62.35765000
O	22.74518000	17.13235000	58.33085000
O	14.88981000	18.99648000	60.08468000
O	16.83659000	20.71378000	64.69926000
O	15.30760000	21.03235000	62.35777000
O	17.21744000	18.99641000	67.17543000
O	17.33095000	18.99646000	62.77465000
O	15.25169000	20.86067000	58.33095000
O	17.13661000	20.87738000	60.67202000
O	18.99846000	18.99650000	60.01357000
O	21.16035000	20.71379000	64.69923000
O	18.99850000	21.30958000	62.46348000
O	20.77967000	18.99642000	67.17533000
O	20.66601000	18.99647000	62.77456000
O	18.99843000	20.96204000	58.39454000
O	20.86034000	20.87738000	60.67200000
O	18.99857000	18.99646000	65.25883000
O	23.10711000	18.99650000	60.08462000
O	22.68937000	21.03237000	62.35769000
O	22.74517000	20.86069000	58.33089000
O	15.01498000	22.69248000	59.99716000
O	18.99846000	22.90289000	59.97140000
O	22.98192000	22.69252000	59.99706000
O	18.99857000	18.99652000	69.48236000

8.2.2. Optimized geometries of cationic $(\text{TiO}_2)_n$ with $n = 4, 8, 16, 35, 84$ in vacuum at B3LYP/6-31G(d) level. $(\text{TiO}_2)_{4a}$

Ti	2.01889200	-0.04217400	0.66046300
Ti	-0.00340900	-1.39853100	-0.92882400
Ti	0.11399200	1.46134500	-0.93398900
Ti	-2.03205500	-0.06313100	0.63902000
O	2.50230900	-0.03803200	2.16782700
O	1.57143600	-1.71132500	-0.23063800
O	1.73186000	1.65790500	-0.40366700
O	-0.01964000	0.11494600	0.44223400
O	0.01972500	0.09785800	-2.06312900
O	-1.84042900	1.70527200	-0.38226200
O	-1.61958200	-1.69335300	-0.25739400
O	-2.44285100	-0.09091100	2.17550100

 $(\text{TiO}_2)_{4b}$

Ti	-2.22645700	0.34960900	0.41488600
Ti	2.58037700	0.15540200	-0.44102100
O	0.98395100	-0.87530900	0.59287400
O	-3.64163100	1.39570200	-0.01146100
O	3.92780700	-0.62823500	-0.18254800
O	1.36735700	-0.43011300	-1.90170100
Ti	0.43430000	0.73941200	1.32743300
O	-1.86878000	-1.12429400	-0.54788700
Ti	-0.03630500	-0.82428400	-0.95817900
O	-1.35071800	0.59407500	1.96463900
O	-0.47873300	0.92326600	-0.33698800
O	1.94325700	1.48228600	0.89358400

 $(\text{TiO}_2)_{4c}$

Ti	-1.60820800	0.00000000	0.83138600
Ti	1.60820800	0.00000000	0.83138500
O	0.00000000	0.00000000	1.72009300
O	-2.94057300	0.00000000	1.80956900
O	2.94057300	0.00000000	1.80956900
O	1.36509900	-1.46061600	-0.42820900
Ti	0.00000000	1.58748500	-1.46879700
O	0.00000000	0.00000000	-2.35157400
Ti	0.00000000	-1.58748500	-1.46879700
O	-1.36509900	-1.46061600	-0.42820900
O	-1.36509900	1.46061600	-0.42820900
O	1.36509900	1.46061600	-0.42820900

 $(\text{TiO}_2)_{4d}$

Ti	-1.18356800	1.80882300	-0.87071000
Ti	0.13899300	0.06970800	-2.45244200
O	-0.60539800	-1.86427800	0.74356200
O	-1.59291200	0.39081900	-1.85239600
O	0.35222200	0.15745200	-4.25435000
O	0.88576600	-1.32904200	-1.64146200
Ti	-0.35089700	-0.17774000	1.75460900
O	0.45058500	1.66304500	-1.54108300
Ti	0.97844600	-1.91385500	0.10849800
O	-1.13965900	1.33403000	0.77180300
O	1.46070700	-0.58245900	1.06266100
O	-0.52754900	-0.27988100	3.33097900

 $(\text{TiO}_2)_{8a}$

Ti	-3.25198200	-0.14730500	0.00002900
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Ti	-0.94629200	1.35386300	-1.80532500
Ti	-0.94625600	1.35375400	1.80542700
Ti	0.76181000	2.68610000	0.00007400
Ti	0.90733200	-1.34871300	1.79171800
Ti	3.16066500	0.11796100	-0.00002800
Ti	0.90729600	-1.34860600	-1.79181700
Ti	-0.78981900	-2.73225200	-0.00007400
O	0.33089700	-1.15901400	-0.00003800
O	-2.58667300	0.94979500	-1.49501400
O	-4.82867600	-0.33466300	0.00003900
O	-0.32836200	1.14329100	0.00003800
O	-0.04811100	2.98669100	-1.58043900
O	-2.58664300	0.94970200	1.49512500
O	-0.04808000	2.98659600	1.58062000
O	2.34344500	1.73936400	0.00003000
O	-0.01013400	-0.01612900	2.56908700
O	2.61220900	-0.89762300	1.43670600
O	4.95107900	0.40028200	-0.00003800
O	2.61218000	-0.89753600	-1.43681300
O	-0.01018700	-0.01597600	-2.56908700
O	-2.29136300	-1.88783300	-0.00003400
O	0.04284000	-2.94092300	1.64738200
O	0.04280700	-2.94082400	-1.64755900
(TiO ₂) _{8b}			
Ti	-1.38656900	-1.23175100	0.54498600
Ti	2.15718500	1.00292600	0.73187300
Ti	1.34746300	-2.48955300	0.04736400
O	1.28914500	-0.54131300	-0.06596300
Ti	-0.01410200	1.37210400	-1.43282900
Ti	2.48789400	-0.47401200	-1.61854200

Ti	-3.34523000	0.33941700	-0.84900400
O	2.01246800	0.39540200	2.41159200
O	-3.32941500	0.55310700	-2.56039100
O	-0.40860400	-2.64637900	-0.16758700
O	-3.47272500	2.03171600	-0.56558800
O	-0.61920800	-0.91014100	2.20614600
O	-3.84137700	3.51300400	-3.24610600
O	1.78726900	-2.45932500	1.76746100
O	-3.10166000	-1.21186400	0.38715400
O	0.98992600	-1.51168100	4.60015500
Ti	-2.94656600	2.48748200	-2.41772100
O	0.95248200	2.08100600	0.00899900
O	-1.32623800	0.23275000	-0.63959900
O	1.24103400	0.44395100	-2.48776300
Ti	1.04048200	-1.11443800	2.83327300
O	2.46342100	-2.28103100	-1.40471900
O	3.44462700	0.60231400	-0.51777600
O	-0.94896500	2.50115600	-2.29306000

(TiO₂)_{8c}

Ti	-2.21937200	-1.56469600	0.89288700
Ti	3.15853600	1.16893800	-0.04201900
Ti	1.01952900	0.41798900	1.65158400
O	-2.61756700	-0.84388200	2.52402300
Ti	-3.04353500	0.98105000	-0.58775000
Ti	2.04791400	-1.34751000	-2.01985900
Ti	-1.87182900	0.79215000	2.24469800
O	3.95080100	2.48438600	-0.45885200
O	-4.46610200	1.70513000	-1.43531900
O	1.93740400	-2.94493300	-1.10959800

O	-3.31169500	-0.85697400	-0.31224000
O	2.67354300	0.91512800	1.80798700
O	-2.87579200	1.74931800	1.08939000
O	-1.06389100	-0.07531800	0.77621700
O	-1.05308000	-2.94634400	0.53088200
O	-1.64126700	1.20017100	-1.71568400
Ti	0.08349800	0.63169800	-1.53727100
O	-0.18497400	1.16501600	2.81945700
O	0.35351000	-1.16130100	-1.06541600
O	1.23245300	-1.45870900	1.48601500
Ti	0.68239900	-2.51731000	0.19202800
O	1.14069700	1.27700500	-0.14656700
O	3.23280500	-0.46947500	-1.17349000
O	1.15083200	0.20433600	-2.86197100

(TiO₂)_{8d}

Ti	3.17298100	0.10283400	-0.67872800
Ti	-1.15549800	0.07809900	-2.59260200
Ti	-1.25905900	-2.54019000	1.81072500
Ti	0.75488600	1.99651800	-1.70795200
O	4.97797500	0.08132700	-0.54665800
O	-0.67679600	0.65966400	1.13569200
O	0.18690700	-1.53280600	2.77022300
Ti	-2.46161400	0.19351000	0.50696600
Ti	0.68466800	-0.58108500	1.44266100
Ti	0.71641000	-1.66421300	-1.47556200
Ti	-1.12885800	2.61656400	1.12811300
O	2.53121200	1.57758200	-1.50795600
O	-2.42901800	0.09789200	-1.38443000
O	-0.72636400	3.34029700	2.48742900

O	-1.56733700	-4.08413100	2.03985000
O	-0.42936100	-1.60121800	-2.86661400
O	0.02382800	2.91236300	-0.45524300
O	2.43631900	-1.37296500	-1.62587300
O	-2.89467900	1.81283700	0.99858000
O	2.39972100	-0.10867500	0.93366700
O	0.24993100	0.16096800	-1.26288200
O	-2.66523100	-1.34617400	1.37721600
O	0.07854400	-1.99672700	0.26005900
O	-0.42710000	1.65513300	-3.09753400

(TiO₂)_{16a}

Ti	3.29358600	-1.59768600	1.45073200
Ti	2.36943100	0.36630700	-2.70312900
Ti	-0.33166200	1.54657400	-2.42747500
Ti	1.70059800	0.46390000	3.37063600
Ti	1.89391900	2.57050300	1.58260900
Ti	1.56155200	-5.28373200	-2.21402800
Ti	0.46634200	-0.42819600	-0.09013400
Ti	-1.34750500	-1.21846300	-2.71941100
Ti	-1.18454800	-2.99509900	1.79955400
Ti	1.37007900	-2.64155300	-3.23568500
Ti	1.79503900	-3.88538200	0.31136900
Ti	-2.92866000	-1.70716900	-0.42727400
Ti	-3.53061500	1.18360200	1.51366800
Ti	3.87316100	1.02437100	-0.41959600
Ti	-1.29299500	-0.67873100	3.32110500
Ti	-0.98328700	2.94890700	-0.01709000
O	-2.64491600	-3.09002300	0.74988700

O	4.37230700	-0.45912600	0.51180800
O	0.15273800	0.00695100	4.18069300
O	-3.57719400	-0.18686000	0.31567600
O	-2.61459200	0.47872100	2.93196100
O	0.46027900	3.51293600	0.96758400
O	-3.04254600	-1.84413000	-2.20316500
O	0.15303400	-6.01411300	-2.36672000
O	1.26276800	-3.38958100	-1.50117700
O	-2.53370800	2.55433300	0.84269400
O	-5.13886200	1.69684100	1.97310700
O	2.21600600	2.21501300	3.34171000
O	0.26473100	-3.95498100	1.37358300
O	1.92347400	-4.18156900	-3.79497600
O	-1.63287900	-2.45274800	3.49145800
O	2.18471900	-5.42680000	-0.37516300
O	3.37030800	-3.35019500	1.23038300
O	2.55517900	-1.23515400	-3.49431900
O	3.39737700	2.49833600	0.60500300
O	2.86996700	-0.87883800	3.09304500
O	4.05615600	1.02155000	-2.20051900
O	-0.39933100	-2.31663600	-3.73235800
O	-0.95868400	3.19864900	-1.79340100
O	2.16961100	0.51799900	-0.77199300
O	-1.14004700	-1.38649700	-0.75100300
O	-0.42516700	1.25494700	-0.42786800
O	1.69995900	-1.66019100	0.49643100
O	0.49195600	-0.42254800	-2.06807500
O	-0.65276200	-1.15486900	1.65097900
O	1.25189000	1.69075100	-3.29892300
O	-1.57998500	0.54336100	-3.22330900

O	1.22006200	0.80765400	1.60608600
(TiO ₂) _{16b}			
O	0.01324000	0.02225200	0.07452900
Ti	0.01541200	-0.02451300	1.93071800
O	1.74394700	0.04944200	2.48501400
O	0.08162200	-2.08546700	-2.29342100
Ti	0.75204400	-0.62299800	-1.43057100
O	-1.01921500	1.26090800	2.70468200
O	-0.51576300	-1.68472000	2.39264700
O	2.25238000	0.23314100	-2.01565000
O	4.44956300	-2.14600400	-1.88977800
Ti	3.48161900	-0.81702500	-1.15349300
O	1.99026800	-1.82129300	-0.68845800
O	0.33761500	-5.17690400	-1.99585600
O	0.02098800	-3.52884000	0.20874900
Ti	0.79190000	-3.53564600	-1.41924700
O	0.38357600	-4.76075000	2.82089000
O	4.26866200	-1.95461800	3.04866400
Ti	0.39370600	-3.19027300	1.91693300
O	2.18029300	-2.74417700	1.91253500
Ti	3.08525300	-1.08836500	2.02122800
O	3.91461100	-0.41287500	0.54527800
O	4.54770400	-3.60083000	0.66306700
Ti	4.19233000	-3.71409600	2.42570700
Ti	5.05187100	-6.45149000	2.53119600
O	3.20056000	-5.45450300	2.50456500
Ti	1.48022100	-6.10535000	2.27766600
O	5.46845500	-4.72746200	3.12331700
O	5.82326900	-7.82095100	3.41184800

Ti	5.09864900	-9.34058300	2.61807900
O	3.54318000	-10.16226700	3.18222900
O	1.35282000	-7.72770500	3.05538100
Ti	2.36104600	-9.08382500	2.33163800
O	3.84547600	-8.06359400	1.90986700
O	3.52962700	-7.18912200	-0.79693500
Ti	1.61189500	-6.28309600	-1.26153700
O	1.22490000	-6.32861000	0.50656000
O	1.41647700	-7.94661700	-1.88983000
O	1.93038100	-9.53193400	0.66080800
O	5.77488600	-9.95842700	1.15533400
O	3.92879200	-9.96282200	-1.42597700
Ti	2.67862200	-8.90185900	-0.89821600
O	6.23755200	-8.13723800	-1.33874100
O	5.77637700	-6.40789600	0.92319600
Ti	5.79617800	-9.96582200	-0.81918300
Ti	5.35453200	-6.75563700	-0.81263600
O	2.58685400	-4.44114000	-1.35221900
Ti	4.31489500	-3.81169100	-1.12599200
O	6.71936300	-11.09197100	-1.46788800
O	5.36680500	-5.11609900	-1.70131300

(TiO₂)_{16c}

Ti	-1.77762100	1.54575700	-2.24393700
Ti	-1.77775000	-1.54499000	-2.24468100
Ti	1.77762100	1.54575700	-2.24393700
Ti	1.77775000	-1.54499000	-2.24468100
Ti	-1.73094200	2.97599800	0.75061200
Ti	1.73094200	2.97599800	0.75061200
Ti	-1.73100700	-2.97610600	0.74938000

Ti	1.73100700	-2.97610600	0.74938000
Ti	-1.65820500	1.34220300	3.40898400
Ti	-1.65811700	-1.34355500	3.40846600
Ti	1.65820500	1.34220300	3.40898400
Ti	1.65811700	-1.34355500	3.40846600
Ti	1.38341700	4.48420200	-1.89077200
Ti	1.38341700	-4.48352800	-1.89251300
Ti	-1.38341700	4.48420200	-1.89077200
Ti	-1.38341600	-4.48352800	-1.89251300
O	2.22156400	-3.19427200	-2.89556300
O	2.22125300	3.19520000	-2.89446100
O	-2.22156400	-3.19427200	-2.89556300
O	-2.22125300	3.19520000	-2.89446100
O	-2.51940200	-2.57714300	2.31413800
O	-2.51927500	2.57649000	2.31523800
O	2.51940200	-2.57714300	2.31413800
O	2.51927500	2.57649000	2.31523800
O	2.07170900	-4.52157000	-0.23055100
O	-2.07173600	4.52180800	-0.22884300
O	2.07173600	4.52180800	-0.22884300
O	-2.07170900	-4.52157000	-0.23055100
O	-2.38439400	-0.00090400	4.42370700
O	2.38439400	-0.00090400	4.42370700
O	-2.59162300	0.00050600	-2.75365600
O	2.59162300	0.00050600	-2.75365600
O	0.00000000	-2.95520300	1.24414700
O	0.00000000	2.95486700	1.24569800
O	0.00000000	-1.05785400	-2.67773900
O	0.00000000	1.05885700	-2.67739600
O	2.00824500	-1.64779800	-0.47919700

O	-2.00838000	1.64820000	-0.47842900
O	2.00838000	1.64820000	-0.47842900
O	-2.00824500	-1.64779800	-0.47919700
O	0.00000000	-3.32582000	-1.48467600
O	0.00000000	3.32644100	-1.48299500
O	0.00000000	5.59039400	-2.39230700
O	0.00000000	-5.58959600	-2.39438000
O	-1.28645300	-0.00043000	2.26612300
O	1.28645300	-0.00043000	2.26612300
O	0.00000000	1.81003200	3.99846200
O	0.00000000	-1.81225000	3.99752100

 $(\text{TiO}_2)_{16d}$

Ti	3.07247800	0.82757700	1.34630000
Ti	-0.35003300	4.34475200	2.00570400
Ti	-1.23606800	0.69078400	5.02345400
Ti	1.58507600	1.59601400	3.63582300
Ti	0.00735000	-0.17080100	0.61880200
Ti	-2.39836400	-1.11317100	-1.96107300
Ti	2.77042900	-2.28325100	0.23113900
Ti	-1.91317500	1.89876900	1.87866200
Ti	2.05764200	-2.18176800	-3.14570000
Ti	0.43645500	-3.56651500	1.22188400
Ti	0.93739600	2.58662800	-0.40841600
Ti	-0.76686400	-4.09892600	-2.05128200
Ti	-1.87393800	-1.71933700	3.06864100
Ti	0.39370000	0.69010900	-2.65585000
Ti	-0.32836000	3.31527700	4.67441300
Ti	-3.19578200	-0.59118600	0.69862100
O	-1.57179700	-0.96504200	-0.26900800

O	1.35829400	0.45217200	1.86844000
O	-0.64383400	-2.97575000	2.64081900
O	3.65601300	-0.84168200	0.92473100
O	2.97447800	-2.33189200	-1.50537100
O	-3.92332200	-0.82049400	-0.92517800
O	0.71745900	-3.25121000	-2.95794700
O	0.68278800	2.50425000	-2.17064500
O	-2.03457100	-0.97955500	4.70955600
O	3.29884300	1.49416200	3.02679700
O	-2.14374400	-2.75466800	-2.36526500
O	-0.99131000	2.18581800	6.03579300
O	3.00170600	-2.86990900	-4.51872600
O	1.51256900	-0.40384600	-3.48119700
O	2.26672700	-3.80055300	1.12287100
O	0.63627500	4.18929900	0.46949400
O	-1.13262100	-5.50791800	-2.70083100
O	-1.31079400	0.12502300	-2.81975500
O	2.63122700	2.09931600	0.12918500
O	-0.38703200	-4.24936400	-0.11936800
O	1.40743000	2.93016000	4.88662400
O	-3.37249100	-1.82188200	2.03264700
O	-1.87154700	1.87941800	3.77720700
O	-0.60545300	1.68537900	0.47030800
O	-3.38421000	1.17740500	1.19581800
O	-1.95421000	3.73096600	1.63014500
O	-0.51500100	4.89812400	3.78872500
O	0.46877400	0.41805700	4.48974200
O	-1.33757400	-0.20253100	2.08345500
O	0.92554500	-1.86547700	0.51463300
O	0.20899800	2.71739500	2.78359200

O 0.87215200 0.29575700 -0.92414400

8.2.3. Optimized geometries of anionic $(\text{TiO}_2)_n$ with $n=4, 8, 16, 35, 84$ in vacuum at B3LYP/6-31G(d) level. $(\text{TiO}_2)_{4a}$

Ti	2.00709300	-0.00004800	0.68746500
Ti	-0.00001300	-1.30046400	-0.85943500
Ti	-0.00006100	1.30073100	-0.85911000
Ti	-2.00697400	-0.00012300	0.68771500
O	2.99073300	-0.00019200	1.99705500
O	1.74252500	-1.57917800	-0.33540500
O	1.74249900	1.57930600	-0.33501400
O	0.00006400	-0.00009400	0.74675400
O	-0.00011900	0.00023700	-2.17232300
O	-1.74256600	1.57924100	-0.33479700
O	-1.74247500	-1.57924300	-0.33518800
O	-2.99045600	-0.00030200	1.99742400

 $(\text{TiO}_2)_{4b}$

Ti	-2.29917700	0.38610400	0.40469400
Ti	2.57155100	-0.09296400	-0.26924500
O	0.93760300	-0.88947600	0.61130500
O	-3.76764600	1.08876800	0.22656300
O	4.04025400	-0.79522400	-0.09149000
O	1.53574000	-0.36328900	-1.85644200
Ti	0.35507300	0.87414900	1.13404300
O	-1.80213400	-1.14210900	-0.63637100
Ti	-0.08265000	-0.58166800	-0.99798100
O	-1.26365400	0.65621200	1.99207900
O	-0.66490400	1.18200900	-0.47554800
O	2.07437000	1.43500400	0.77202400

$(\text{TiO}_2)_{4c}$

Ti	-1.61367700	0.00000000	0.85799100
Ti	1.61367700	0.00000000	0.85799100
O	0.00000000	0.00000000	1.76480000
O	-2.95850900	0.00000000	1.79187300
O	2.95850900	0.00000000	1.79187300
O	1.44755300	-1.48597700	-0.42117500
Ti	0.00000000	1.41633100	-1.40098300
O	0.00000000	0.00000000	-2.57786300
Ti	0.00000000	-1.41633100	-1.40098300
O	-1.44755300	-1.48597700	-0.42117500
O	-1.44755300	1.48597700	-0.42117500
O	1.44755300	1.48597700	-0.42117500

 $(\text{TiO}_2)_{4d}$

Ti	-0.90121800	1.31229900	-0.69703500
Ti	0.20595600	0.04479800	-2.79713400
O	-0.77852400	-1.67980800	0.80183300
O	-1.54719400	0.23058000	-1.93257400
O	0.34830000	0.21372500	-4.41995700
O	0.98298100	-1.42379000	-1.91848500
Ti	-0.39482700	-0.16535700	1.99041500
O	0.58958000	1.55933800	-1.60862800
Ti	0.71233800	-1.43286200	-0.10968800
O	-1.17172900	1.30330500	1.11178200
O	1.35835400	-0.35124900	1.12591800
O	-0.53728200	-0.33435700	3.61322100

 $(\text{TiO}_2)_{8a}$

Ti	-3.19224700	-0.16807700	0.00001600
Ti	-0.87073500	1.28447600	-1.78441200
Ti	-0.87071900	1.28446200	1.78445600
Ti	0.77607300	2.71091700	0.00008500
Ti	0.87076200	-1.28458000	1.78436000
Ti	3.19224300	0.16807600	-0.00003700
Ti	0.87070200	-1.28437300	-1.78450000
Ti	-0.77607500	-2.71091100	-0.00006100
O	0.25937800	-1.14223700	0.00003000
O	-2.55866500	0.87649000	-1.51326500
O	-4.80414900	-0.29654800	0.00004200
O	-0.25937600	1.14224300	0.00010000
O	-0.03375600	2.98615400	-1.62498400
O	-2.55861500	0.87650200	1.51336400
O	-0.03383500	2.98608600	1.62522900
O	2.36507400	1.93636500	0.00005400
O	0.00001800	-0.00008400	2.76162900
O	2.55865300	-0.87658800	1.51326000
O	4.80414400	0.29655600	-0.00003700
O	2.55863900	-0.87639000	-1.51337100
O	-0.00004100	0.00008400	-2.76181800
O	-2.36508400	-1.93635100	-0.00001600
O	0.03386900	-2.98620300	1.62503900
O	0.03372300	-2.98607100	-1.62515200

(TiO₂)_{8b}

Ti	-1.23794300	-1.24393800	0.52375800
Ti	2.04205300	0.91618800	0.71087400
Ti	1.36293700	-2.52598000	0.12088200
O	1.10939000	-0.62705000	0.02486500

Ti	-0.02268000	1.49759200	-1.50912000
Ti	2.36022700	-0.50157300	-1.57434600
Ti	-3.17201600	0.34500300	-0.85132500
O	2.04170000	0.46689500	2.42499900
O	-3.34078900	0.57494000	-2.59306500
O	-0.43860100	-2.77976200	-0.10448900
O	-3.45394900	2.05773100	-0.55871400
O	-0.69056400	-0.98054600	2.16846300
O	-3.89119900	3.55071000	-3.23525900
O	1.86976100	-2.58410900	1.80077800
O	-3.03967000	-1.15346600	0.30274200
O	1.13256100	-1.47758700	4.48809000
Ti	-2.97980600	2.49100700	-2.40756500
O	0.90875600	2.15109700	-0.08880800
O	-1.26235400	0.28735400	-0.72106300
O	1.17777400	0.55608600	-2.52844000
Ti	1.10936700	-1.15268400	2.90321900
O	2.51005500	-2.39114700	-1.27667100
O	3.42763000	0.57486300	-0.36569700
O	-1.04990700	2.63322500	-2.38175400

(TiO₂)_{8c}

Ti	-2.22671100	-1.56695700	0.82748200
Ti	3.14575100	1.15258700	-0.12792900
Ti	1.07661400	0.41810700	1.64939600
O	-2.62359700	-0.84021100	2.47323400
Ti	-3.15248000	1.01816100	-0.64231700
Ti	2.11072700	-1.27370600	-1.93547200
Ti	-1.82497200	0.78799700	2.15807500
O	4.00239500	2.48421900	-0.47698500

O	-4.48222800	1.64252000	-1.31337300
O	1.96964100	-2.93120700	-0.90324200
O	-3.35211200	-0.93494000	-0.34753700
O	2.77193900	0.85500100	1.76406000
O	-2.84210200	1.80309700	1.15735900
O	-1.04149200	-0.08098600	0.69753000
O	-1.12933400	-3.03003300	0.57019500
O	-1.61922900	1.24727700	-1.78084400
Ti	-0.02239600	0.55120600	-1.44145000
O	-0.14220200	1.18667100	2.81299100
O	0.13144900	-1.32154000	-1.23566300
O	1.17663100	-1.42970200	1.50588600
Ti	0.59346100	-2.44638700	0.13903400
O	1.12841300	1.25683400	-0.08573600
O	3.48090300	-0.36119800	-1.20673600
O	1.18575100	0.31905400	-2.70882500

(TiO₂)_{8d}

Ti	3.25102800	0.07192000	-0.72770700
Ti	-1.07001700	0.04503300	-2.43959700
Ti	-1.22584900	-2.52825000	1.73500100
Ti	0.77355700	1.93948600	-1.58037300
O	4.86411400	0.09179100	-0.61039900
O	-0.70651100	0.71490100	1.21752500
O	0.15405400	-1.54551800	2.65989400
Ti	-2.42998300	0.21662600	0.54762300
Ti	0.66245500	-0.63156300	1.22793400
Ti	0.85756700	-1.79135000	-1.57631700
Ti	-1.13596800	2.64203400	1.12921800
O	2.51576900	1.69627000	-1.52179600

O	-2.47528400	0.04538500	-1.29055700
O	-0.88163900	3.56015500	2.43807200
O	-1.53412400	-4.06758800	2.14796200
O	-0.50628700	-1.53440000	-2.97697200
O	-0.01190700	2.99569400	-0.37972700
O	2.58453700	-1.46302500	-1.70869200
O	-2.91344800	1.88109900	0.95188700
O	2.35000100	-0.18393100	0.97709300
O	0.29615700	0.13541500	-1.11291300
O	-2.69000100	-1.32113400	1.43387100
O	-0.00871800	-2.11898000	0.19840200
O	-0.32703900	1.60733600	-3.05028400

(TiO₂)_{16a}

Ti	3.33861200	-1.61483300	1.53072400
Ti	2.33450000	0.36531400	-2.69758400
Ti	-0.34224600	1.59382200	-2.49168100
Ti	1.68041100	0.45922200	3.36073900
Ti	1.87553400	2.52186300	1.53610100
Ti	1.47382600	-5.10553400	-2.13301600
Ti	0.43133300	-0.47475900	-0.08598500
Ti	-1.42968900	-1.15218000	-2.74390500
Ti	-1.18409800	-3.04360300	1.79025200
Ti	1.24092900	-2.47618900	-3.14622500
Ti	1.82800800	-3.78665200	0.41975900
Ti	-2.98135100	-1.74272100	-0.45865900
Ti	-3.50363500	1.15545700	1.49900700
Ti	3.86140100	0.94615300	-0.41559700
Ti	-1.28554800	-0.75136200	3.33238000

Ti	-0.95181800	2.95480500	-0.08981300
O	-2.61549300	-3.16465900	0.71167400
O	4.44738500	-0.48826000	0.55659900
O	0.17880900	-0.04818300	4.21881000
O	-3.70549100	-0.33835700	0.29443900
O	-2.57074000	0.37551300	3.02181100
O	0.51395100	3.54264600	0.93840800
O	-3.11294100	-1.80903300	-2.27763800
O	0.21374300	-6.10206800	-2.31409300
O	1.08912500	-3.28412100	-1.40758700
O	-2.44398500	2.61148200	0.76095700
O	-4.94952800	1.70268700	1.95776600
O	2.17979500	2.23118700	3.32488500
O	0.31133600	-4.03336000	1.43336900
O	1.83997100	-4.03837300	-3.69742800
O	-1.66736100	-2.55975700	3.48030600
O	2.31686200	-5.26671900	-0.42163700
O	3.42765900	-3.38822600	1.41928200
O	2.54234400	-1.20509600	-3.55853800
O	3.41693800	2.45706200	0.59064500
O	2.93496700	-0.81632600	3.17342800
O	4.07221800	0.99622600	-2.19806600
O	-0.49422600	-2.28715300	-3.77663300
O	-0.97725100	3.23888900	-1.90718600
O	2.19599300	0.42205200	-0.77287800
O	-1.23418600	-1.31667700	-0.80750800
O	-0.35184700	1.31168300	-0.57187400
O	1.81235800	-1.74405800	0.60654000
O	0.48872500	-0.45328000	-2.19324800
O	-0.65126700	-1.24965000	1.66126000

O	1.29279400	1.73712100	-3.31783900
O	-1.62706200	0.60124400	-3.28703400
O	1.19651600	0.77810100	1.60748200

(TiO₂)_{16b}

O	-0.21901500	0.02163000	0.07703400
Ti	-0.05369600	-0.05653000	1.96963300
O	1.88039600	0.09044300	2.27800700
O	0.35968200	-2.24497600	-2.27474100
Ti	0.77394800	-0.63524400	-1.25175500
O	-0.93726200	1.05199000	2.74666100
O	-0.37714100	-1.88204700	2.58354600
O	2.35052600	0.23980500	-2.10031800
O	4.47145300	-2.10535500	-1.94005700
Ti	3.58330000	-0.61794600	-1.20237300
O	2.31145400	-1.54003600	-0.20154300
O	0.31033800	-5.37655500	-1.98460800
O	0.12177700	-3.53822800	0.30128200
Ti	0.75785800	-3.69572300	-1.37478500
O	0.44314500	-4.95944800	2.87617400
O	4.46129700	-1.70212200	2.64277500
Ti	0.52199500	-3.27239400	2.04265700
O	2.31147600	-2.85312600	2.15310000
Ti	3.08497600	-0.90300500	1.55096800
O	4.13022100	0.08393300	0.37925000
O	4.54990200	-3.55530700	0.61293200
Ti	4.16287100	-3.40451800	2.36671500
Ti	5.00031400	-6.16477200	2.58671700
O	3.21757600	-5.63619100	2.47186900
Ti	1.49464900	-6.26437400	2.28274400

O	5.40681300	-4.54098600	3.22454400
O	5.36025300	-7.78419400	3.39297300
Ti	4.87491300	-9.24801700	2.41126800
O	3.48234700	-10.22725800	3.12448300
O	1.27561900	-7.93801100	3.02245100
Ti	2.11857800	-9.35987600	2.25845000
O	3.50476300	-8.43334500	1.37983100
O	3.55029600	-7.06995600	-0.88566700
Ti	1.63619900	-6.38844700	-1.25006900
O	1.22142900	-6.45050400	0.50778400
O	1.48005800	-8.13115900	-1.68750400
O	1.58746400	-9.88370100	0.65902100
O	5.91921800	-9.92556700	1.18546100
O	3.93278800	-9.95516000	-1.17572700
Ti	2.72481500	-8.90361400	-0.53768300
O	6.24004900	-8.04347000	-1.31372300
O	5.69967600	-6.34297200	0.95484500
Ti	5.84670900	-9.83892400	-0.76381800
Ti	5.32397400	-6.62834400	-0.80726300
O	2.54294300	-4.41614900	-1.35197500
Ti	4.26397900	-3.70808800	-1.16573000
O	6.75108100	-10.95448300	-1.49681000
O	5.37943400	-5.01904000	-1.71164200

(TiO₂)_{16c}

Ti	-1.71914000	1.57995500	-2.28374700
Ti	-1.71920500	-1.57947800	-2.28373600
Ti	1.71914000	1.57995500	-2.28374700
Ti	1.71920500	-1.57947800	-2.28373600
Ti	-1.69799600	3.00467900	0.71562100

Ti	1.69799600	3.00467900	0.71562100
Ti	-1.69811100	-3.00435800	0.71586300
Ti	1.69811100	-3.00435800	0.71586200
Ti	-1.63875000	1.34163600	3.31309200
Ti	-1.63878100	-1.34125800	3.31323000
Ti	1.63875000	1.34163600	3.31309200
Ti	1.63878100	-1.34125800	3.31323000
Ti	1.36763400	4.52685700	-1.81472600
Ti	1.36799900	-4.52704700	-1.81492400
Ti	-1.36763500	4.52685700	-1.81472600
Ti	-1.36799900	-4.52704700	-1.81492400
O	2.18633600	-3.27055500	-2.88276700
O	2.18652200	3.26987000	-2.88311200
O	-2.18633600	-3.27055500	-2.88276700
O	-2.18652200	3.26987000	-2.88311200
O	-2.54202300	-2.57230200	2.29070500
O	-2.54199500	2.57221500	2.29091900
O	2.54202300	-2.57230200	2.29070500
O	2.54199500	2.57221400	2.29091900
O	2.15773600	-4.56778300	-0.14485500
O	-2.15793700	4.56774600	-0.14410200
O	2.15793700	4.56774600	-0.14410200
O	-2.15773600	-4.56778300	-0.14485500
O	-2.40813200	0.00006100	4.32428300
O	2.40813200	0.00006100	4.32428200
O	-2.50426500	-0.00032900	-2.80486400
O	2.50426500	-0.00032900	-2.80486400
O	0.00000000	-2.98709100	1.36508300
O	0.00000000	2.98724700	1.36531800
O	0.00000000	-1.32265400	-2.75311300

O	0.00000000	1.32278600	-2.75337100
O	1.97314800	-1.67749300	-0.48897400
O	-1.97323400	1.67747600	-0.48910300
O	1.97323400	1.67747700	-0.48910400
O	-1.97314800	-1.67749300	-0.48897300
O	0.00000000	-3.44491800	-1.24079800
O	0.00000000	3.44399400	-1.24004000
O	0.00000000	5.67016200	-2.37737200
O	0.00000000	-5.66955900	-2.37739600
O	-1.26907700	-0.00005700	2.17458200
O	1.26907700	-0.00005700	2.17458200
O	0.00000000	1.79654200	3.99463400
O	0.00000000	-1.79617900	3.99471700

(TiO₂)_{16d}

Ti	3.02679500	0.81682300	1.35949300
Ti	-0.30751900	4.29799600	2.00612800
Ti	-1.19023600	0.68332400	4.95826400
Ti	1.55716800	1.63408200	3.68696900
Ti	0.03023900	-0.16150400	0.59013700
Ti	-2.38112700	-1.15252300	-1.93385800
Ti	2.76167400	-2.27703000	0.24606600
Ti	-1.91031600	1.92450300	1.87184200
Ti	2.10435900	-2.15354500	-3.17487600
Ti	0.40749700	-3.55643600	1.20230400
Ti	0.93382500	2.61137500	-0.41459100
Ti	-0.75076100	-4.08927000	-2.06615200
Ti	-1.86312600	-1.70871500	3.05968300
Ti	0.37219900	0.67758000	-2.65675900
Ti	-0.37086200	3.29661800	4.70011200

Ti	-3.17697500	-0.58065300	0.71363400
O	-1.56894000	-1.00000100	-0.24708700
O	1.33466700	0.39616600	1.85431700
O	-0.67697600	-3.01732600	2.66367900
O	3.68199200	-0.83372700	0.95048900
O	3.04922500	-2.36344900	-1.43533900
O	-3.92520500	-0.80586100	-0.91108500
O	0.63251400	-3.18820800	-2.84903700
O	0.66557900	2.51026300	-2.18432000
O	-2.02789900	-1.00424700	4.72087300
O	3.28214600	1.50910500	3.02128800
O	-2.23107300	-2.80329400	-2.35291500
O	-1.01132000	2.07031200	6.07932900
O	3.01431200	-2.70404600	-4.39603800
O	1.50021800	-0.27013500	-3.54308400
O	2.23304300	-3.81946500	1.15142300
O	0.66319800	4.22757200	0.38220800
O	-1.05999700	-5.52151800	-2.75747900
O	-1.35677500	0.07776000	-2.85079800
O	2.63231100	2.10883600	0.13785000
O	-0.42493700	-4.30393000	-0.09608000
O	1.44924600	2.92046800	4.92986800
O	-3.39680800	-1.81200700	2.05374200
O	-1.89638700	1.91559400	3.76927900
O	-0.61055200	1.69158100	0.43891500
O	-3.40275900	1.17642200	1.19675100
O	-1.98775700	3.71683300	1.64240900
O	-0.37578900	5.02397000	3.61229300
O	0.52603700	0.34516600	4.49150100
O	-1.34759900	-0.20707900	2.08894300

O	0.89508200	-1.88653200	0.49023300
O	0.23221900	2.68469300	2.73453200
O	0.90385900	0.26934200	-0.93079000