

## **Understanding the Nature and Location of Hydroxyl Groups on Hydrated Titania Nanoparticles**

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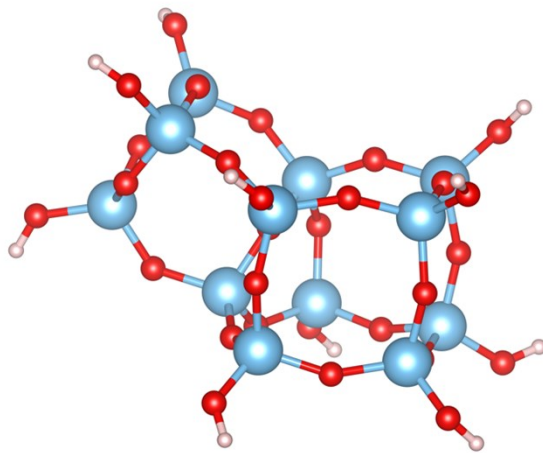
### **Contents**

(TiO<sub>2</sub>)<sub>12</sub>(H<sub>2</sub>O)<sub>5</sub> NP model (Fig. S1)

Scaled frequencies of surface hydroxyl groups (Table S1)

XYZ coordinates of the hydrated TiO<sub>2</sub> NPs

**Fig. S1** Structure of the  $(\text{TiO}_2)_{12}(\text{H}_2\text{O})_5$  nanocluster. The free hydroxyl (OH) groups are connected to Ti atoms which have tetrahedrally connectivity. Blue, white and red spheres correspond to Ti, H, and O atoms, respectively.



**Table S1.** Scaled frequencies of the Surface hydroxyl (OH) groups of (TiO<sub>2</sub>)<sub>35</sub>(H<sub>2</sub>O)<sub>13</sub>, (TiO<sub>2</sub>)<sub>35</sub>(H<sub>2</sub>O)<sub>30</sub>, (TiO<sub>2</sub>)<sub>84</sub>(H<sub>2</sub>O)<sub>24</sub>, and (TiO<sub>2</sub>)<sub>84</sub>(H<sub>2</sub>O)<sub>55</sub> NPs depicted in Fig. 4.

(TiO <sub>2</sub> ) <sub>35</sub> (H <sub>2</sub> O) <sub>13</sub>		(TiO <sub>2</sub> ) <sub>35</sub> (H <sub>2</sub> O) <sub>30</sub>		(TiO <sub>2</sub> ) <sub>84</sub> (H <sub>2</sub> O) <sub>24</sub>		(TiO <sub>2</sub> ) <sub>84</sub> (H <sub>2</sub> O) <sub>55</sub>	
Frequency [cm <sup>-1</sup> ]	IR-intensity [D <sup>2</sup> /Ang <sup>2</sup> ]	Frequency [cm <sup>-1</sup> ]	IR-intensity [D <sup>2</sup> /Ang <sup>2</sup> ]	Frequency [cm <sup>-1</sup> ]	IR-intensity [D <sup>2</sup> /Ang <sup>2</sup> ]	Frequency [cm <sup>-1</sup> ]	IR-intensity [D <sup>2</sup> /Ang <sup>2</sup> ]
3273.719853	8.47817435	3134.465326	0.1981586	3391.350814	12.46771675	2976.080864	6.93119631
3342.290937	7.33863892	3160.750529	0.19982033	3392.2084	3.34479275	3011.839065	30.52950462
3516.744953	5.64928855	3222.364748	0.20371554	3399.370298	8.71287063	3064.485254	14.85536893
3568.066769	1.44598861	3225.252016	0.20389807	3497.442559	8.35909835	3095.896681	25.79350945
3656.022293	1.67386109	3298.635436	0.20853731	3541.416498	3.32320996	3112.951602	7.09219149
3656.271975	3.07015818	3302.002496	0.20875018	3556.782872	2.27987107	3155.061565	6.69589247
3659.351184	2.07874484	3323.902461	0.21013468	3572.580995	8.4993366	3157.967958	20.89539066
3667.979646	3.55359557	3347.242533	0.21161022	3575.829569	6.1586022	3172.891632	7.22479772
3672.817554	5.37029784	3363.004171	0.21260666	3579.392194	2.10232386	3176.951271	9.2190924
3673.229611	1.73391292	3416.186276	0.21596879	3580.275001	2.92886571	3196.598504	6.26769125
3673.412608	5.42084693	3518.910796	0.22246296	3584.916383	1.80272158	3205.175879	9.2989558
3675.293584	4.2496583	3528.122964	0.22304535	3600.476478	4.05803219	3244.817336	11.69493209
3675.894581	2.56113013	3540.006857	0.22379664	3616.587754	2.56620016	3249.134721	7.7474787
3679.970923	3.21877801	3560.267923	0.22507753	3632.130897	7.6664249	3254.551101	4.57227853
3681.373223	4.59774363	3560.983378	0.22512276	3632.570646	1.33897586	3275.991584	11.2623157
3682.792379	3.53269879	3572.369875	0.2258426	3647.591862	1.46805653	3292.329032	9.91751432
3683.854112	4.27901337	3574.791666	0.22599571	3649.383373	2.66944216	3317.711344	7.50532996
3684.290856	5.34886793	3587.590895	0.22680486	3649.981347	2.07983572	3372.664449	3.82440443
3685.209449	4.22212271	3594.220659	0.22722399	3660.619596	1.35115148	3398.912685	3.90929948
3688.165703	3.8868558	3602.477498	0.22774598	3661.34083	4.13901673	3401.394684	3.23139263
3689.931815	3.4694389	3602.56022	0.22775121	3661.439395	3.96619476	3401.701494	7.23041525
3692.032137	3.23673734	3619.321788	0.22881087	3664.023394	1.71277316	3408.524021	8.50689897
3695.891003	1.36794823	3631.564126	0.22958482	3665.499959	4.50263781	3410.52909	1.58288007
3696.937408	7.8643059	3634.52058	0.22977173	3665.822619	1.13889176	3473.039323	6.65303349
3706.794151	5.80068328	3637.508782	0.22996064	3668.441578	1.2962612	3474.04422	4.37062163
3707.804306	3.64038177	3645.737768	0.23048087	3669.235074	2.63528974	3483.200116	2.39407691
		3650.091314	0.2307561	3672.753762	4.47689407	3510.506685	3.53763437
		3651.849395	0.23086724	3674.203145	3.57055157	3532.089203	2.63699024
		3652.347535	0.23089873	3674.504831	7.97162277	3540.171321	1.39759971
		3652.474284	0.23090675	3674.683012	0.39637594	3557.340354	5.07449742
		3661.676249	0.23148849	3675.691914	2.78992553	3559.243934	1.83382691
		3662.906785	0.23156628	3676.702232	0.42759676	3560.994651	0.97040903
		3666.908014	0.23181923	3677.505057	0.29240412	3569.383027	1.62220039
		3668.503213	0.23192008	3677.563685	5.99733611	3572.756756	1.22296094
		3669.641641	0.23199205	3677.714741	2.89753743	3578.857576	1.27167863
		3672.781206	0.23219053	3678.15498	11.91913519	3583.484774	1.78658006
		3673.151741	0.23221396	3680.858212	3.65426528	3591.785	1.50858977
		3673.955867	0.2322648	3683.036484	4.70073044	3595.34564	2.3072054
		3675.590737	0.23236815	3684.121508	5.0943139	3596.328125	1.26904105
		3680.12077	0.23265494	3686.153855	4.30262144	3603.082821	1.20693009
		3682.216023	0.232787	3689.896829	5.5766396	3604.537979	1.49476621
		3682.768433	0.23282192	3690.430825	2.71444857	3605.023711	3.25651556
		3684.006331	0.23290018	3695.731354	3.18863681	3609.599151	1.31917969
		3686.512676	0.23305863	3704.303112	4.20029555	3612.045391	0.72750937
		3689.362005	0.23323876	3705.144872	5.21029855	3623.881475	1.70979103
		3689.540491	0.23325004	3706.100574	5.92412743	3628.82928	2.65418673
		3689.815488	0.23326743	3717.484613	17.12866833	3631.977013	4.66272313
		3691.848269	0.23339594	3717.797244	0.75732741	3632.109758	2.10427605
		3694.105224	0.23353862			3632.498341	1.40018807
		3695.721045	0.23364077			3636.167142	2.48397622
		3696.363365	0.23368138			3637.150614	1.87181438
		3697.260846	0.23373812			3640.262911	1.09977268
		3698.067853	0.23378914			3648.138258	3.65468937
		3699.029283	0.23384992			3650.004535	2.02884587
		3700.376455	0.23393509			3651.427548	1.66404245
		3701.802335	0.23402523			3652.092195	1.00945957
		3705.658211	0.23426899			3652.196992	2.92793396
		3713.022121	0.23473453			3653.425497	1.45426423
		3714.951149	0.23485649			3653.951154	0.27694952
		3728.654302	0.23572279			3655.05407	4.01561864
						3655.87012	1.73110767
						3656.149688	3.25796908
						3656.83058	3.16281198
						3658.062224	0.90987688
						3661.051398	0.22487892
						3661.711454	2.46073462
						3663.824999	5.3442251
						3664.358485	3.16719953
						3665.39885	1.97256619
						3667.156411	4.81134848
						3667.26117	0.07313749
						3668.351599	3.35700308
						3668.763368	2.3913026
						3668.802963	0.33004299
						3669.649416	6.8359256
						3670.465594	1.88306523
						3671.412592	0.63639745
						3671.444599	2.51333797
						3671.842988	2.69944006
						3673.834838	2.6496095
						3674.112	5.20939694
						3674.72968	2.70076482
						3675.162842	5.82048444
						3675.563012	1.88432756
						3677.19185	5.71934502
						3677.678324	2.80652071
						3677.914652	3.04955018
						3679.213722	0.78225566
						3680.083818	2.16214185
						3680.672101	4.79337405
						3681.48301	4.35934737
						3683.095144	3.85825295
						3683.855221	3.9455797
						3684.432472	3.92014269
						3686.122496	3.84218293
						3686.477466	2.70490607
						3686.90383	0.26350357
						3688.093003	3.23339372
						3689.671902	1.14068277
						3690.11612	7.8064214
						3692.988172	3.62638061
						3693.268974	4.15523731
						3695.14384	3.42489693
						3695.792328	3.65258788
						3695.997824	4.62580127
						3697.997463	4.84945654
						3701.301893	1.10175011
						3702.320063	7.60832739
						3716.335778	8.0530576
						3716.69939	7.18945285

XYZ files of TiO<sub>2</sub> NPs(TiO<sub>2</sub>)<sub>12</sub>(H<sub>2</sub>O)<sub>5</sub>

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PBE xc

H	-1.17742654	-4.53806909	-5.72575897
O	-0.69329209	-4.54842491	3.80343812
H	-6.39649210	-3.48071486	-3.45463221
H	1.71519733	-6.68527617	-1.60805749
O	-2.36918347	-3.00204372	1.85430685
H	-0.39566494	-5.46547885	3.90987716
H	2.57274497	0.45813675	4.15300422
O	-4.15334679	-0.65055193	-2.29093023
H	1.04177399	0.95929271	-5.24692456
H	-6.31762935	0.11537811	4.75014264
O	-4.54700277	-0.95886114	2.23747323
H	4.75043523	-0.68757259	-0.63254719
H	-1.34869832	3.88425019	4.69808792
O	-2.84999668	1.03447966	3.59314090
H	-5.22295591	4.89613237	0.03050508
Ti	-0.66440349	-3.50556850	2.31501623
Ti	-4.54292386	-2.43052510	-2.04480955
Ti	0.81172130	-4.46587542	-0.75305836
Ti	-1.46429986	2.02881731	2.95515719
Ti	-4.55284533	0.68224709	3.00073154
Ti	-1.47186233	-3.64506094	-3.36951589
Ti	-3.75314144	2.90372213	0.65464359
Ti	2.29761852	-1.22924985	-1.00043646
Ti	1.11789878	-0.40126614	2.26605597
Ti	-2.91062953	0.35418504	-1.41643460
Ti	-3.49976101	-1.86266013	1.02427098
Ti	-0.12186000	-0.35299984	-3.41202880
O	-3.20048456	-3.37691594	-2.80289352
O	-3.56048226	1.97962785	-0.91182412
O	-2.53856088	-0.59518038	0.11302857
O	1.78249461	-5.99203120	-0.93305563
O	-4.88858433	1.93206416	1.69814701
O	-6.16069600	-2.85811699	-2.74966732
O	-0.49153035	-4.38587863	-2.00597695
O	0.21588697	0.53968130	-4.95845668
O	0.06297934	-4.39594342	0.92257860
O	-0.87201976	3.17981730	4.23176892
O	1.88065515	-3.00306562	-0.94000202
O	-0.75026640	-2.05254617	-3.78196874
O	1.36495962	-0.49255953	-2.41352040
O	-1.44979019	-4.74507609	-4.81779930
O	-4.37119858	4.59051442	0.37945626
O	4.08176328	-1.00276702	-1.26093746
O	-1.41303873	0.49350840	-2.43880109
O	0.30432104	-1.98883123	2.61656910
O	-5.76411199	0.80415567	4.35017491
O	-2.14419063	2.94247360	1.52761023
O	-4.50516676	-2.71774181	-0.22969041
O	2.51097277	-0.16125688	3.40850218
O	-0.06937148	0.94795865	2.46286205
O	1.78071078	-0.47001658	0.54721145

**(TiO<sub>2</sub>)<sub>35</sub>(H<sub>2</sub>O)<sub>13</sub>**

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PBE xc

O	20.16903542	18.68735227	38.03927740
Ti	16.88762869	17.00296094	43.80097235
Ti	16.92006277	15.27915896	46.19565241
O	16.97173116	17.06714711	46.10199349
O	16.91993370	14.95201251	48.33556715
O	16.57990477	15.24801527	44.39690258
O	16.80764953	16.87691795	42.02023121
O	15.08073607	14.91434773	46.76348496
Ti	20.47065849	16.85019768	43.67947517
Ti	18.60050779	17.17127227	41.38059218
Ti	20.65465619	15.24360288	46.07142955
O	20.55046030	17.00336839	45.90239641
O	18.67905292	17.18540303	43.71498204
O	20.65511702	14.74556686	48.20958485
O	20.70715620	15.09767464	44.23616936
O	18.52104038	16.89975260	39.59074275
O	20.38429053	16.72491302	41.88338279
O	18.73214981	14.78538889	46.53901285
O	22.46988259	15.08536308	46.48942159
Ti	17.19008984	20.73889301	43.79087066
Ti	16.76120264	18.93806522	46.27599091
O	17.11190694	20.78773602	45.93236662
O	16.97782972	18.97181903	48.35326639
O	16.52277099	18.90128492	44.29739592
O	16.86488548	20.87198486	41.99804920
O	15.00966003	19.04112879	46.81084052
Ti	18.61502337	18.66677080	38.98945346
Ti	21.06859338	20.59087781	43.64267962
Ti	18.60506034	20.99222248	41.38345218
Ti	20.80462833	18.94624420	46.11092606
O	18.66050853	18.92437683	41.00810844
O	20.78757909	20.73453188	45.57321268
O	18.91983298	20.59219468	43.39175865
O	20.83049516	18.83581837	48.15291880
O	21.06006433	18.69893677	44.08764552
O	18.64771842	20.71164888	39.41666650
O	20.66101970	20.80739062	41.70967873
O	18.87165047	18.95487463	46.59596161
O	22.71083395	18.89853568	46.53669845
Ti	17.14763438	22.58911715	46.02285547
O	17.21018077	23.00663089	48.17648570
O	16.95674480	22.59915611	44.23030259
O	15.33586103	23.01825984	46.58810475
Ti	20.87021205	22.87775536	46.00449192
O	20.91827944	22.83565730	47.97347738
O	20.92794366	22.58723338	44.00234659
O	18.98212703	22.96115644	46.35548521
O	22.83335589	22.31994011	46.41906490
Ti	15.07001019	15.35845946	48.88866018
Ti	17.24159032	17.29194712	53.47047897
Ti	15.39855999	17.19988307	51.18080475
O	15.20898008	15.39925212	50.70072316
O	17.22318478	17.32973237	55.25833751
O	15.43756841	17.09376716	53.00392175

O	14.77264028	17.20094209	48.97708836
O	17.18496616	17.28827631	51.19277029
Ti	18.79396488	15.17625526	48.63098389
Ti	20.97491562	17.31727367	53.25315243
Ti	19.00418634	16.90715928	50.88653811
O	18.91088767	15.10246236	50.45588014
O	21.20712467	17.13586378	55.05603132
O	19.08223506	16.75735631	52.87904436
O	18.89327296	16.96852780	48.79634720
O	20.89045417	17.13032332	51.09894593
Ti	22.51515922	15.05018229	48.30067878
Ti	22.67680050	16.97503419	50.91983187
O	22.93516341	15.11382452	50.44372820
O	22.77102403	16.88430796	52.71965789
O	22.88117080	16.90226476	48.74635987
Ti	15.19987760	19.05505837	48.65687272
Ti	17.32454606	20.86879119	53.37030949
Ti	15.57998562	20.97132633	51.07469297
Ti	17.67462462	19.13556437	55.75390241
O	14.97919061	19.08184996	50.70301411
O	17.29041226	20.91297507	55.16986771
O	15.54816524	21.15027677	52.90154851
O	17.52177591	19.18701981	57.56103601
O	17.58145413	19.06857392	53.45430247
O	14.93396668	20.94037927	48.94942289
O	17.33607148	20.75718236	51.15207204
Ti	18.92898620	18.89973964	48.50865799
Ti	21.09039150	21.20254079	53.07290006
Ti	19.27133905	20.89786501	50.79591125
Ti	21.47454865	18.91073036	55.50601470
O	19.11773346	18.93680850	50.41131776
O	21.39324655	20.95421014	55.02744368
O	19.18288736	21.32204411	52.81573473
O	21.33697123	19.12182120	57.47986347
O	20.97680193	19.08141362	53.51579501
O	19.03714253	20.82492311	48.75733078
O	21.07542624	20.71856847	51.21858867
O	19.45000906	19.11946806	56.00993086
Ti	22.63100005	18.78865600	48.32509542
Ti	23.29824827	20.61809553	50.67570738
O	23.24307819	18.73355628	50.45956961
O	23.06681042	20.87407761	52.66101894
O	22.91833939	20.63820299	48.79515383
Ti	15.37597672	22.77535836	48.76485716
O	15.52838886	22.78198240	50.56349198
Ti	19.07230303	22.61851474	48.51960021
O	19.25756773	22.76050774	50.29867461
Ti	22.91791383	22.79508225	48.39035610
O	22.83857991	22.64155158	50.32465149
Ti	19.32568402	19.21808752	58.04065964
O	19.40287025	17.84378855	59.23397381
H	18.89153262	17.01988090	59.17418256
O	19.48703302	20.82133505	58.89066836
H	18.71536782	21.35032905	59.15549335
H	20.64435204	17.87479267	37.79587109
O	17.17619285	18.74425894	37.87509970
H	16.32725969	18.29392617	38.01756825

O	24.79542768	22.70069177	48.35923023
H	25.27139183	22.61966928	47.51548636
H	22.32686006	23.11319353	51.01376988
O	23.61079836	13.56250801	48.43062382
H	23.77179054	13.08935980	47.59513509
H	22.99623940	14.35397078	51.04413475
O	13.54591672	14.31845255	48.83280822
H	13.09722718	14.17784241	49.68533760
H	14.31101307	14.88992467	46.17234646
H	14.55188880	23.04625771	46.01682900
O	13.98964936	23.99299773	48.66708692
H	13.59140569	24.24734364	49.51834519
H	22.08511269	18.98520030	58.08345359
O	23.30745742	18.88380396	55.49376899
H	23.76571417	18.09691636	55.14574319
O	21.33516484	23.03597814	52.97484827
H	20.53808409	23.57902505	52.83172018
H	21.55127599	21.66732479	55.66728144
H	23.78034549	20.94158413	53.31674332
O	25.06136068	20.96692956	50.59652092
H	25.30902176	21.61709373	49.89033407
O	18.68427817	22.81643931	41.27656458
H	17.97626797	23.34759036	41.68555849
H	18.50619498	21.42453594	38.77278684
H	21.34307908	20.85797958	41.02025679
O	22.87745733	20.61344611	43.39734071
H	23.41518329	19.81724070	43.55219411
O	21.32621404	24.60914276	45.84152563
H	21.87501151	24.94467942	46.59978051
H	21.07060914	23.28358956	43.34019727
O	22.84928443	24.65415010	48.15457940
H	23.71058779	25.10319474	48.22374809
H	22.97744719	21.37400549	46.21624476

**(TiO<sub>2</sub>)<sub>35</sub>(H<sub>2</sub>O)<sub>30</sub>**

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PBE xc

O	-9.70640156	-3.77194615	0.71595160
Ti	-4.74733315	1.13755116	2.23342542
Ti	-2.33353092	0.95633593	4.33353257
O	-2.88812616	1.12350612	2.12500229
O	-0.49021231	1.34744550	4.03224332
O	-4.42843135	0.91588769	4.26587183
O	-6.90887546	0.95515667	1.99947108
O	-2.42220780	3.04643748	4.04930842
Ti	-4.38426138	-2.79588415	1.83625709
Ti	-6.97420081	-1.03166116	2.45386690
Ti	-1.75174564	-2.68265790	3.69894045
O	-2.40024315	-2.51768410	1.81318165
O	-5.13769598	-0.83844546	2.21412774
O	0.12888940	-2.28885314	3.71327551
O	-3.80080030	-3.06041470	3.72468721
O	-8.92990763	-1.72464316	2.57019844
O	-6.30910168	-2.93592265	2.49184127
O	-1.87491123	-0.80897905	4.02557140
O	-1.04426506	-4.49264358	2.98972346
Ti	-5.14163140	1.36826214	-1.54793857

Ti	-2.65800810	1.53973408	0.25443697
O	-3.22380940	1.50275929	-1.65027958
O	-0.58651741	1.81036587	0.17507318
O	-4.62923374	1.38735577	0.36609066
O	-7.14795624	0.98966576	-0.78489480
O	-2.46099721	3.42190060	0.33803812
Ti	-9.47265129	-1.96057878	0.66359520
Ti	-4.50737783	-2.42539405	-1.78688376
Ti	-7.29950108	-0.86497398	-1.39840035
Ti	-2.05882843	-2.23874962	-0.08769443
O	-7.68736062	-1.27441077	0.53768304
O	-2.62875933	-2.20001792	-1.95258187
O	-5.44568514	-0.55974855	-1.79380913
O	-0.02737343	-1.88787369	-0.26242248
O	-4.07779314	-2.14088166	0.04945897
O	-9.19523493	-1.80626419	-1.29400475
O	-6.51197443	-2.71590899	-1.71137124
O	-1.88717911	-0.29737063	0.01383678
O	-1.25656685	-4.01642277	-0.24741147
Ti	-2.75948161	1.77096214	-3.62146057
O	-0.87238863	2.05749891	-3.76566897
O	-4.89721044	1.56101878	-3.55769177
O	-2.68515623	3.75863039	-3.02666754
Ti	-2.27910825	-1.90728393	-4.04679404
O	-0.35025234	-1.60995022	-4.05895429
O	-4.25791291	-2.29279116	-3.79074352
O	-2.28843436	-0.03024489	-3.78552376
O	-1.57151621	-3.84394383	-3.87474218
Ti	-0.55465518	3.56257277	4.17193117
Ti	4.51018748	2.43624584	2.00948978
Ti	1.75726382	4.10658416	2.15447134
O	1.46747055	3.39388949	4.06541922
O	6.44370102	2.90409229	1.82251432
O	3.78327842	4.30513554	2.11148981
O	-0.20839476	3.82796729	2.18856709
O	2.55373534	2.15764435	1.89415187
Ti	0.28489494	-0.36680238	3.59782233
Ti	5.04731834	-1.28517728	1.59434781
Ti	2.48678889	0.25653497	1.80194287
O	2.05219560	0.00655705	3.67262711
O	7.06077344	-0.75303383	1.59627026
O	4.42552656	0.55343673	1.73693718
O	0.43432977	-0.18104613	1.81228042
O	3.19794750	-1.60346740	1.50841739
Ti	0.90450508	-4.33830258	3.44784529
Ti	3.07549327	-3.70350966	1.25677770
O	2.78226828	-3.59629154	3.36461654
O	5.10669335	-3.27147282	1.15481065
O	1.16076293	-3.95538926	1.36696796
Ti	-0.63505150	3.60623184	0.30601608
Ti	4.27319591	2.80574037	-1.99922849
Ti	1.59057329	4.41709586	-1.58265190
Ti	6.77196030	3.08763457	-0.17380264
O	1.40391790	4.16724849	0.28612883
O	6.38772377	3.03496145	-2.14045652
O	3.67068005	4.69346746	-1.60996481
O	8.80915221	3.35320096	0.15077882



O	4.94982653	2.68558114	-0.08693539
O	-0.34987965	4.14616022	-1.50476975
O	2.40009256	2.49006450	-1.84281833
Ti	0.03813981	0.01539553	-0.03132032
Ti	4.95057168	-0.88260480	-2.42587420
Ti	2.31204140	0.51073044	-2.06543989
Ti	7.38247864	-0.77846910	-0.38614421
O	1.94844123	0.31407671	-0.11646788
O	6.94365775	-0.69223627	-2.37576861
O	4.25289031	0.86487635	-2.11703273
O	9.41800777	-0.40686532	-0.53249883
O	5.54135647	-0.97061776	-0.39237645
O	0.24430303	0.23617373	-1.91837322
O	3.00063950	-1.26328147	-2.19641953
O	7.69332862	1.27719117	-0.35629698
Ti	0.49879830	-3.60422671	-0.43112555
Ti	2.85451109	-3.33870053	-2.42429511
O	2.69361717	-3.55933134	-0.57423934
O	4.85191009	-2.87923287	-2.50546306
O	0.89328279	-3.69840012	-2.31299816
Ti	-0.83147418	4.30347359	-3.59872108
O	1.14890344	4.11256332	-3.60614695
Ti	-0.11498363	0.30414215	-3.66778231
O	1.66438820	0.56022093	-3.90690140
Ti	0.37959774	-3.50099636	-4.34826095
O	2.23072869	-2.77355151	-4.32236913
Ti	9.56742489	1.58324924	-0.39983081
O	10.92027564	1.56427334	0.82500244
H	10.96138570	1.45773858	1.78750709
O	10.25760159	2.00865715	-2.03485836
H	11.21386591	2.11920189	-2.17143048
H	-9.80483148	-4.31797622	-0.08151319
O	-11.03266520	-1.01099379	0.74050499
H	-11.93371861	-1.37070706	0.77694820
O	0.79335869	-5.31663486	-4.53277569
H	0.65843363	-5.88766859	-3.75535314
H	2.33273937	-1.81295015	-4.47440002
O	0.62716427	-4.57646418	5.20756520
H	-0.19346252	-4.14673367	5.58633742
H	3.35581484	-4.24480234	3.81248993
O	-0.50256381	3.32903957	6.04182305
H	0.35125674	3.32699484	6.50664403
H	-3.15369968	3.35832150	3.46837516
H	-2.83573284	3.86310794	-2.06544317
O	-0.80102092	6.15044338	-3.34491970
H	-1.02407120	6.68473927	-4.12750198
H	10.08950867	-1.10523149	-0.49398994
O	7.94278324	-2.54636320	-0.38178848
H	7.18104673	-3.15700960	-0.32034107
O	5.02410045	-0.60901961	-4.24838174
H	4.62073310	0.19884622	-4.61524320
H	7.46348399	-0.36923539	-3.12767212
H	5.43861390	-3.47601444	-2.99807726
O	3.32002714	-4.97785487	-3.08725932
H	2.80507020	-5.30127145	-3.85658271
O	-7.99599470	-0.38862798	-3.05386238
H	-7.36831357	0.06632094	-3.64535486

H	-9.80606007	-1.51374461	-1.99099227
H	-6.93045677	-3.58149380	-1.58593523
O	-4.47822183	-4.32191014	-1.59124700
H	-3.59002750	-4.67395089	-1.79981845
O	-2.49959490	-2.10726500	-5.84299275
H	-1.68796063	-2.43989804	-6.30147419
H	-4.92464501	-2.26244115	-4.49408390
O	0.04416902	-3.31883872	-6.18371091
H	0.31107500	-4.04396420	-6.77462050
H	-1.96896581	-4.44536476	-4.52888014
H	-9.43457292	-1.74898237	3.39811995
O	-7.16096687	-0.66898257	4.25361162
H	-6.33763307	-0.31309051	4.65055770
O	-5.04291195	2.95555064	2.71198057
H	-5.20096485	3.55412178	1.95932352
H	-7.38393195	1.57908894	2.57493830
H	-4.73379530	1.67464166	4.79732059
O	-2.30980250	1.16777881	6.12845250
H	-1.71904054	1.90895035	6.42084634
O	6.80478369	4.95151753	-0.23887506
H	5.90426555	5.32732757	-0.30037908
H	9.20113143	4.24078061	0.14518366
H	7.06581520	2.93707482	2.56400870
O	4.78760477	2.24747766	3.81707798
H	4.91782996	1.34929836	4.17407689
O	1.68212407	5.82854949	2.71764396
H	0.87481297	6.02590132	3.25619723
H	4.20186140	5.09418499	2.49178042
H	1.80670614	2.47841823	4.13437062
O	-0.62733127	5.42878335	4.26134127
H	-0.73480964	5.78202699	5.16239553
O	-5.83132469	3.08964403	-1.63949362
H	-6.75757788	3.16745681	-1.34958549
H	-7.13857639	1.05669933	0.20762222
O	-3.05870559	2.26731381	-5.41439682
H	-3.92564723	2.12886551	-5.82887382
H	-5.30098158	2.42406200	-3.76921463
H	6.70298260	3.82854013	-2.60399206
O	4.34634229	3.10303579	-3.83391546
H	5.18413918	3.07236065	-4.32287997
O	1.52831459	6.20867671	-1.87031763
H	0.71752968	6.49665749	-2.36465907
H	3.82111955	5.42072412	-2.23974751
H	1.50377047	3.25978100	-3.92545851
O	-1.29188206	4.30036812	-5.33194193
H	-1.94722345	3.63188853	-5.67169864
O	-4.57209127	-4.47459285	1.18729385
H	-4.57193170	-4.60234921	0.19660100
H	-6.82680156	-3.72566623	2.26358869
H	-4.44627370	-2.99607863	4.44588319
O	-1.75980141	-3.39636405	5.44949930
H	-2.45019469	-4.04404994	5.67223409
O	1.50345101	-6.09163837	3.12660443
H	1.34367149	-6.73323322	3.83945811
H	-1.21983838	-4.56609511	2.02761625
H	7.61238620	-1.20812951	2.25246174
O	5.33740632	-1.59226360	3.40867032

H	4.51969635	-1.91434034	3.84088556
O	3.60996583	-5.43183586	1.50525018
H	2.94241364	-5.97799708	1.99624553
H	5.60348364	-3.90972627	1.69411726

**(TiO<sub>2</sub>)<sub>84</sub>(H<sub>2</sub>O)<sub>24</sub>**

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PBEx

O	19.56107896	18.62078274	37.45199887
O	16.78259710	15.09018374	44.27266624
O	16.70572545	17.28143102	42.05263354
O	15.01264715	15.07223571	46.71376899
O	18.99457984	16.76729603	39.59035254
O	19.21469556	20.54023392	39.49252611
O	20.85980782	20.63730557	41.86723358
O	21.07737132	22.62299569	44.16154078
O	22.87140995	22.70132176	46.57252642
O	13.25091505	13.58399175	55.53261466
O	24.78753958	13.36625170	55.44614404
O	13.49027987	24.93157205	51.32864178
O	24.55965118	24.50569381	55.30219732
O	24.75746724	22.77668456	57.75019826
O	22.88953133	24.58789608	48.90833393
O	24.61173530	24.34667262	51.30499252
O	15.09747945	15.34105441	60.26204152
O	17.20444176	17.40233100	64.97819794
O	15.21226524	17.24910132	62.64804496
O	17.31951910	19.07977650	67.31160115
O	20.65730813	21.34602765	64.72473959
O	21.07337031	19.04983056	67.25044737
O	22.96066687	21.08845715	62.45828203
O	19.17539727	18.54440358	69.36050139
O	19.27679885	16.71337886	67.04487757
O	21.42442134	18.41211179	39.72181225
O	12.00830409	25.82129582	53.34936303
O	25.54827866	11.80529731	53.44217226
O	25.98147310	25.61904314	53.29207415
O	12.05755028	12.16808024	53.55713535
O	22.81240923	19.74182545	65.25202615
O	18.82345644	22.55653048	41.16790355
O	23.03023633	20.62909491	43.66164414
O	21.27202246	23.25523399	62.60450578
O	21.00241227	24.71744025	45.92609517
O	24.97602313	21.06942341	60.35840216
O	22.99611891	24.92366670	57.81058328
O	24.90810768	22.73573239	48.59409707
O	26.80562323	22.82580146	55.98724329
O	23.01131415	26.70919263	50.57749359
O	15.33477970	19.51027763	65.57803494
O	18.26267849	15.08144674	41.62807977
O	17.06346903	15.23660727	63.33042345
O	14.69686330	17.09195479	44.20404820
O	13.14803430	17.30946560	60.91700246
O	16.92498712	13.01430257	46.12626402
O	13.02946151	15.09402038	48.66816198
O	15.00065747	13.32084109	58.32006555

H	19.83709365	16.60056615	66.23681235
H	19.08457178	19.25379706	70.01596116
H	18.83949770	18.74254520	36.81509467
H	21.51157628	17.90948104	40.56942216
H	11.57811117	26.06419375	54.18826009
H	12.73635262	24.92637770	50.71765058
H	25.74289980	11.34156198	52.60858506
H	24.80071190	12.61994537	56.06639213
H	26.42477924	25.78004893	54.14520156
H	25.07435259	23.78527516	50.65046820
H	11.78008732	11.73177744	52.73238395
H	13.56148171	12.94858664	56.20411646
H	21.83559252	18.67695811	67.72374980
H	23.14492739	20.47867720	65.79248451
H	19.45421269	21.30544151	38.94502894
H	18.08672375	23.08040117	41.53176592
H	23.56556293	19.87102889	43.95657601
H	21.52804620	20.44213055	41.18653099
H	19.74046616	21.56952948	64.98634606
H	21.73470182	23.66956051	61.84795070
H	20.26954289	25.27728412	46.23974104
H	21.06762651	23.34338275	43.51005455
H	23.33497112	20.36845165	63.00363341
H	25.41680945	20.21117114	60.22396525
H	22.20323973	25.40312804	57.50657919
H	25.39484731	22.54094881	58.45049810
H	23.58416670	22.65751450	45.91424342
H	25.42769664	21.92566460	48.74670897
H	23.95668193	24.91331582	55.96775751
H	27.46322572	22.13332555	55.80899147
H	23.02533471	25.29207660	48.25325119
H	22.34862292	27.40156381	50.73701099
H	16.53893212	18.87256569	67.85091244
H	14.85920524	20.28512307	65.22693468
H	19.36881333	15.99270246	39.13828454
H	17.61218724	14.75010837	40.98564209
H	17.52093487	16.78497362	65.66501979
H	16.37319600	14.80496172	63.85940638
H	16.46960606	18.17563827	41.73406174
H	14.29045064	17.60926506	44.92901088
H	12.54297955	17.70003186	60.25933489
H	14.52301851	17.50147247	63.28559872
H	17.34282178	14.63603822	43.60624953
H	17.27516110	12.41484876	46.81135771
H	12.53780269	14.47102043	49.23690292
H	14.27544395	14.85938633	46.11747159
H	14.92008987	14.60615791	60.86976347
H	15.83777317	12.82571558	58.37326103
O	16.97528651	16.99213746	45.92497583
O	16.92851878	15.13625319	48.19568514
O	20.69111977	17.06626471	46.03000551
O	18.67769427	17.03903161	43.65528464
O	20.66797074	15.20372888	48.42430366
O	20.76949608	15.13511676	44.43953665
O	20.60066229	16.84943724	42.07597718
O	18.89758913	14.84917942	46.69229742
O	22.56502278	14.96169235	46.79628266

O	17.18177585	20.75246171	46.01448613
O	17.01313456	18.98791786	48.39334488
O	16.73421710	18.96350600	44.37572667
O	17.03262799	20.68430799	42.08048913
O	15.09065418	18.91515340	46.80607776
O	18.75198764	18.72461816	40.97442905
O	20.85103996	20.79468452	45.75024336
O	19.08452380	20.65080031	43.48606696
O	20.86509319	18.88970024	48.35202843
O	21.09781264	18.76801096	44.27741116
O	18.93060693	18.91234477	46.76008673
O	22.76174459	18.90279216	46.74870791
O	17.21633038	22.68399976	48.33018352
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O	19.15710113	24.66326801	49.03729470
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O	22.64988849	17.20650888	58.38161690
O	14.98245538	19.23043287	60.18661709
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O	15.41892415	21.19803551	62.41299761
O	17.24589063	19.10820048	63.29533957
O	15.34850622	20.94719758	58.40755245
O	17.25926478	20.96085639	60.74238867
O	19.02974253	19.12533770	60.04591512
O	19.06442432	21.39605959	62.38924913
O	20.91361894	19.36360134	63.15326474
O	19.02413231	21.01839011	58.36525424
O	21.02156740	21.05163230	60.83627643
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O	23.11307499	19.03314976	60.08147027
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Ti	17.34230475	20.79116323	43.89654980
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Ti	19.68093576	18.60575661	39.27231529
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Ti	18.91515870	17.12261360	51.03868389
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Ti	24.53909753	16.99574013	53.33681344
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**(TiO<sub>2</sub>)<sub>84</sub>(H<sub>2</sub>O)<sub>55</sub>**

417

PBE xc

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