Electronic supplementary information (ESI)

Determination of Acid Structures on the Surface of Sulfated Monoclinic and Tetragonal Zirconia through Experimental and Theoretical Approaches

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Table S1. The acid models on SZ.

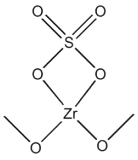
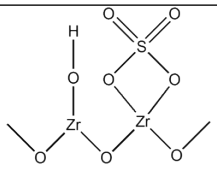
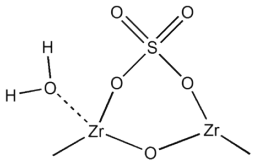
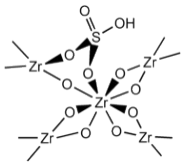
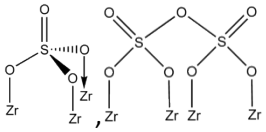
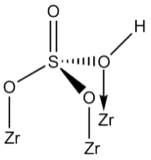
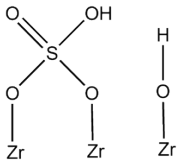
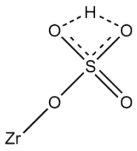
Proposed models	References	Proposed models	References
	Yamaguchi[1]		Ward[2]
	Arata[3]		Clearfield[4, 5]
	Lavalley[6]		Riemer[7]
	Morterra[8]		Kustov[9]

Table S2. The ΔE_{NH_3} on different structures.

Samples	ΔE_{NH_3} (kJ·mol^{-1})		Origin
	Zr-(OH)-Zr	Zr-OH	
S-M(111)	-97, -74		Figure 3a
S-M(-111)	-117, -88		Figure 3b
S-M(001)	-73, -66, -66		Figure 3c
S-M(011)	-67		Figure 3d
S-T(101)	-79, -65		Figure 4a
S-T(001)	-71, -55		Figure 4b
S-T(100)	-76, -65		Figure 4c
S-T(111)-1	-61	-58	Figure 4d
S-T(111)-2	-76		Figure 4e
2S-T(111)	—[a]		Figure 4f

[a] The ΔE_{NH_3} on the hydroxyl groups on 2S-T(111) is out of detection because of the nearby highly acidic protons on Zr-(OH)-SO_2.

Table S3. The unit parameters of the structures on different planes.

Structural models	a (Å)	b (Å)	Angle (degree)	Unit area per H_2SO_4 ($Å^2/H_2SO_4$)
S-M(111)	7.39	7.51	114.6	50.5
S-M(-111)	6.80	7.39	63.73	45.1
S-M(001)	10.37	10.53	90	109.2
S-M(011)	10.37	7.51	83.12	77.3
S-T(101)	6.37	7.26	90	46.2
S-T(001)	7.25	7.25	90	52.6
S-T(100)	10.48	7.26	90	76.1
S-T(111)-1	10.26	6.37	66.28	59.8
S-T(111)-2	10.26	6.37	66.28	59.8
2S-T(111)	10.26	6.37	66.28	29.9

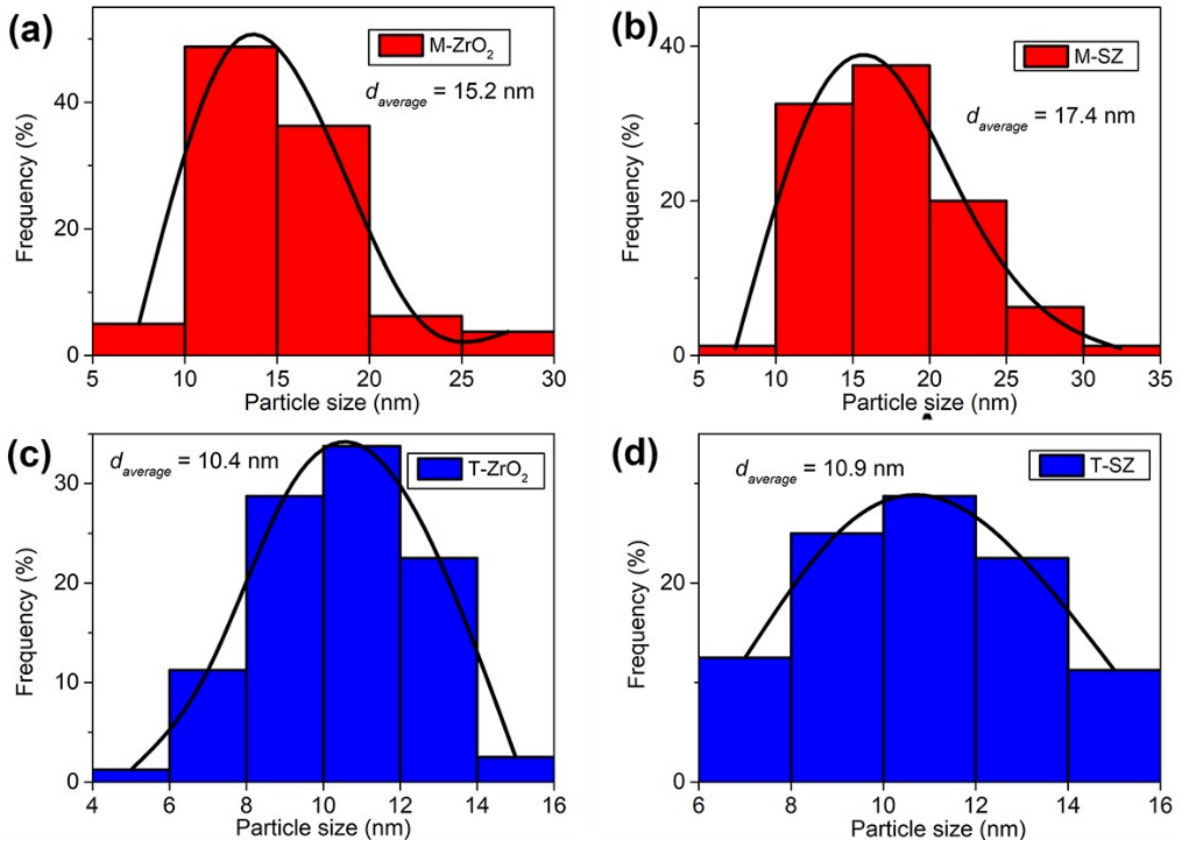


Figure S1. The particle size distributions of (a) M-ZrO_2, (b) M-SZ, (c) T-ZrO_2 and (d) T-SZ.

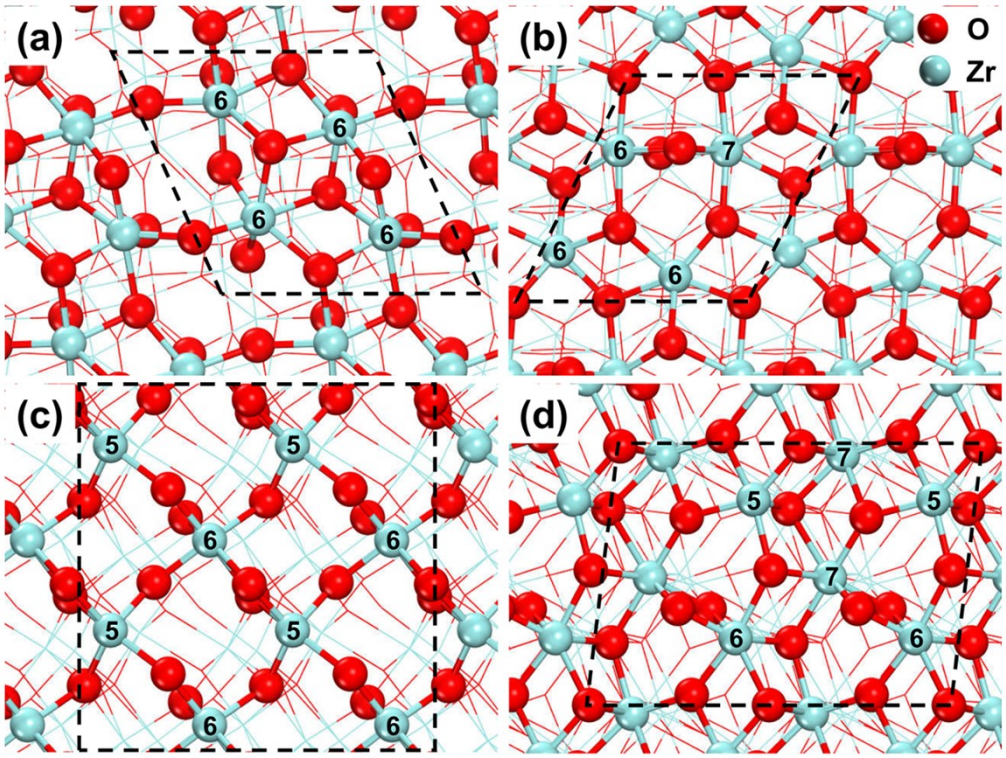


Figure S2. The clean planes of monoclinic zirconia. (a) M(111), (b) M(-111), (c) M(001) and (d) M(011). The numbers on zirconium cations represent their coordination number. The area within the dotted lines corresponds to the unit in Table S3.

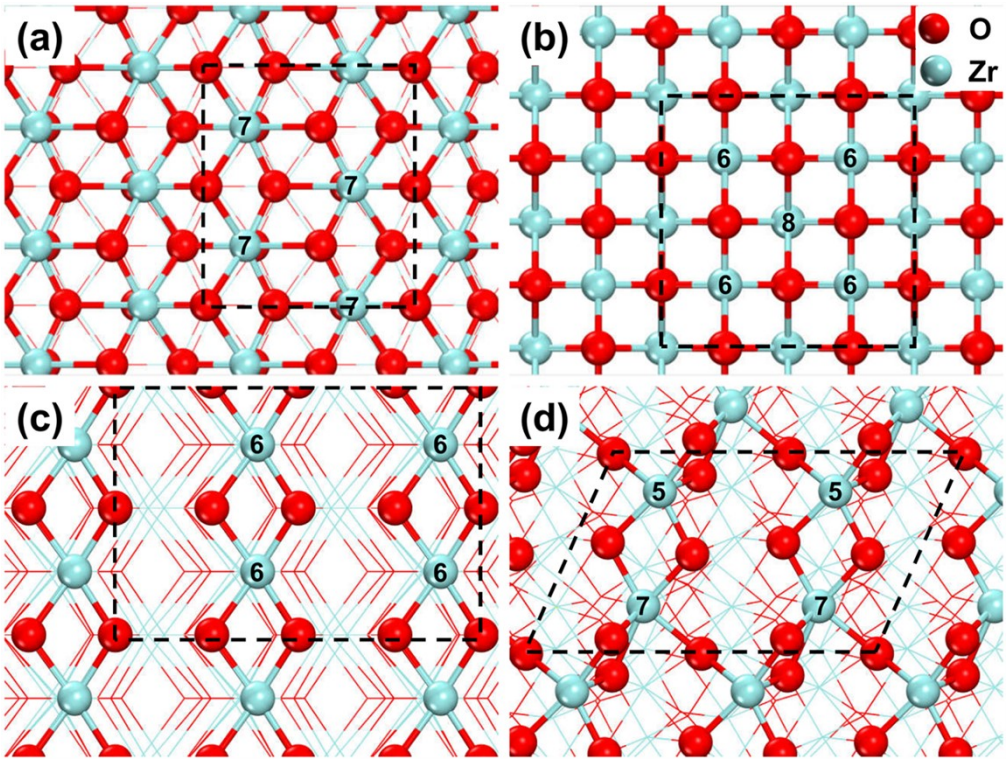


Figure S3. The clean planes of tetragonal zirconia. (a) T(101) (b) T(001), (c) T(100) and (d) T(111). The numbers on the zirconium cations represent their coordination number. The area within the dotted lines corresponds to the unit in Table S3.

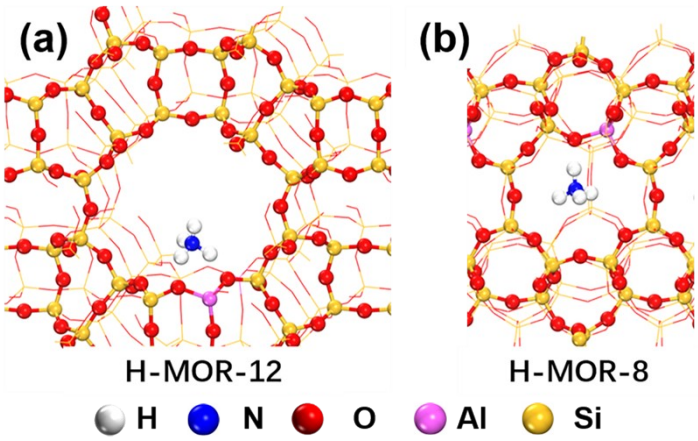


Figure S4. The structures of NH_3 adsorbed on (a) H-MOR-12 and (b) H-MOR-8.

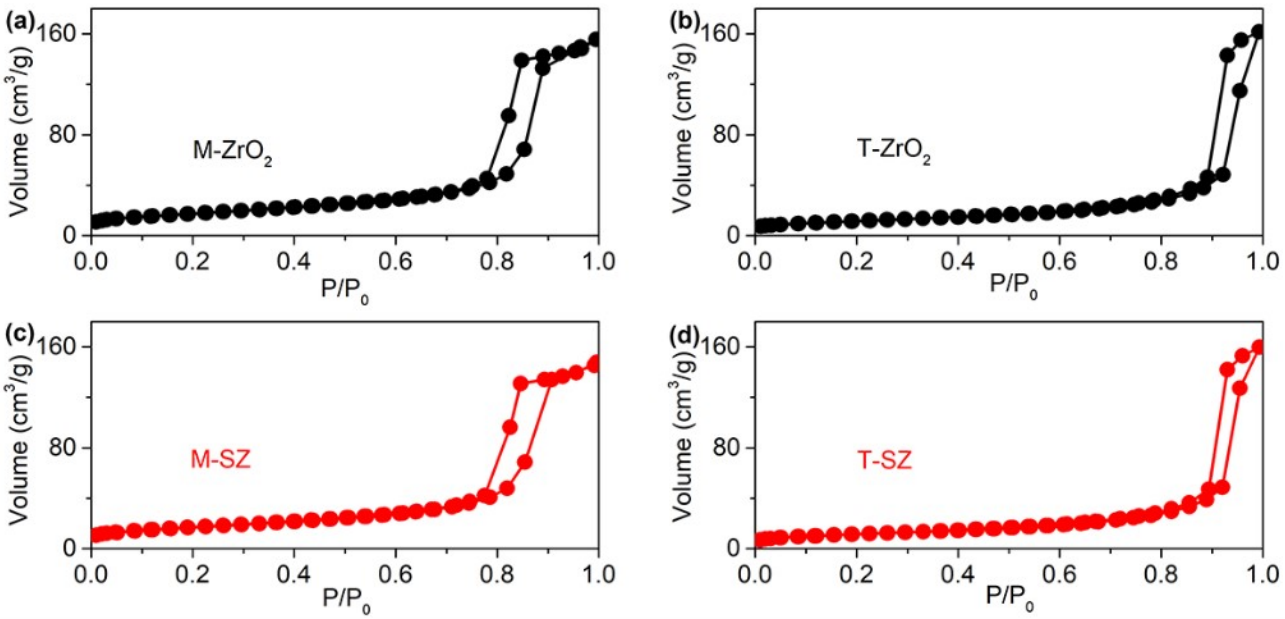


Figure S5. N_2 adsorption-desorption isotherms of (a) M-ZrO_2, (b) T-ZrO_2, (c) M-SZ and (d) T-SZ.

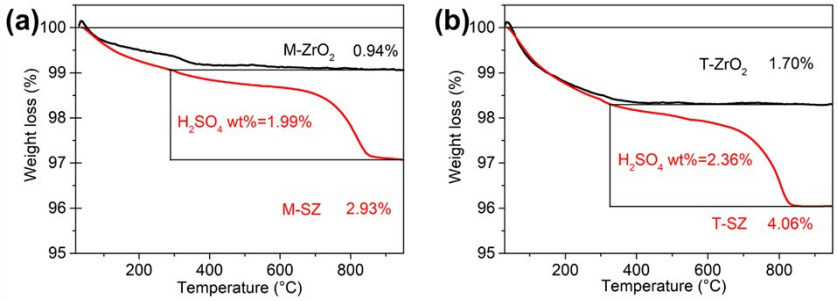


Figure S6. The TG curves of (a) M-ZrO_2 and M-SZ and (b) T-ZrO_2 and T-SZ.

The third step of the weight loss could be corresponded to the chemical dissociation of SO_3 to SO_2 and O_2 species on zirconia.[10] The sulfur content in form of sulfuric acid may be calculated by

$$\mathrm{H2SO4\ wt\%} = \mathrm{SO3\ wt\%} \times \frac{98}{80}$$

as 1.99 wt% for M-SZ and 2.36% for T-SZ.

The calculation of the adsorbed sulfuric acid molecules on M-SZ and T-SZ. (Section 3.5.1)

$$S_{M/T(hkl)} = D(H_2SO_4) \times N_A \times U_{S\text{-}M/T(hkl)} \quad (1)$$

According to the equation (1), for M-SZ, if the strong BA only relates to S-M(001)

$S_{M(001)} = D(H_2SO_4) \times N_A \times U_{S\text{-}M(001)} = 23.9\ \mu mol \cdot g^{-1} \times 6.022 \times 10^{23}\ mol^{-1} \times 109.2\ Å^2 = 15.7\ m^2 \cdot g^{-1}$.

If the strong BA only relates to S-M(011),

$S_{M(011)} = D(H_2SO_4) \times N_A \times U_{S\text{-}M(011)} = 23.9\ \mu mol \cdot g^{-1} \times 6.022 \times 10^{23}\ mol^{-1} \times 77.3\ Å^2 = 11.1\ m^2 \cdot g^{-1}$.

So, the total specific surface area of M(001) and M(011) is in the range of 11.1 ~ 15.7 $m^2 \cdot g^{-1}$ and the specific surface area of the rest crystal planes is 44.5 ~ 49.1 $m^2 \cdot g^{-1}$.

If M(111) represents the rest planes, the sulfuric acid density on M(111) is calculated as

$D(H_2SO_4) = S_{M(111)} / (N_A \times U_{S\text{-}M(111)}) = (44.5 \sim 49.1)\ m^2 \cdot g^{-1} / (6.022 \times 10^{23}\ mol^{-1} \times 50.5\ Å^2)$

$= 146 \sim 161\ \mu mol \cdot g^{-1}$.

If M(-111) represents the rest planes, the sulfuric acid density on M(-111) is calculated as

$D(H_2SO_4) = S_{M(-111)} / (N_A \times U_{S\text{-}M(-111)}) = (44.5 \sim 49.1)\ m^2 \cdot g^{-1} / (6.022 \times 10^{23}\ mol^{-1} \times 45.1\ Å^2)$

$= 164 \sim 181\ \mu mol \cdot g^{-1}$.

As a result, the sulfuric acid density on M(111) and M(-111) is in the range of 146 ~ 181 $\mu mol \cdot g^{-1}$. The percentage of the sulfuric acid molecules related to these strong BA sites is 23.9 / (23.9 + 181) × 100% ~ 23.9 / (23.9 + 146) × 100% = 12 ~ 14%.

For T-SZ, the specific area for T(111) is calculated by equation (1) as

$S_{T(111)} = D(H_2SO_4) \times N_A \times U_{S\text{-}T(111)\text{-}1,2} = 29.2\ \mu mol \cdot g^{-1} \times 6.022 \times 10^{23}\ mol^{-1} \times 59.8\ Å^2 = 10.5\ m^2 \cdot g^{-1}$, and

$S_{T(111)} = D(H_2SO_4) \times N_A \times U_{2S\text{-}T(111)} = 29.2\ \mu mol \cdot g^{-1} \times 6.022 \times 10^{23}\ mol^{-1} \times 29.9\ Å^2 = 5.3\ m^2 \cdot g^{-1}$.

So, the specific area of T(111) is in the range of 5.3 ~ 10.5 $m^2 \cdot g^{-1}$ and the total area of the rest planes is 29.9 ~ 35.1 $m^2 \cdot g^{-1}$.

If T(101) represents the rest planes, the sulfuric acid density on T(101) is calculated as

$D(H_2SO_4) = S_{T(101)} / (N_A \times U_{S\text{-}T(101)}) = (29.9 \sim 35.1)\ m^2 \cdot g^{-1} / (6.022 \times 10^{23}\ mol^{-1} \times 46.2\ Å^2)$

$= 107 \sim 126\ \mu mol \cdot g^{-1}$

If T(001) represents the rest planes, the sulfuric acid density on T(001) is calculated as

$D(H_2SO_4) = S_{T(001)} / (N_A \times U_{S\text{-}T(001)}) = (29.9 \sim 35.1)\ m^2 \cdot g^{-1} / (6.022 \times 10^{23}\ mol^{-1} \times 52.6\ Å^2)$

$= 94.4 \sim 111\ \mu mol \cdot g^{-1}$

If T(100) represents the rest planes, the sulfuric acid density is calculated as

$D(H_2SO_4) = S_{T(100)} / (N_A \times U_{S\text{-}T(100)}) = (29.9 \sim 35.1)\ m^2 \cdot g^{-1} / (6.022 \times 10^{23}\ mol^{-1} \times 76.1\ Å^2)$

$= 65.2 \sim 76.6\ \mu mol \cdot g^{-1}$

So, the sulfuric acid density on the rest planes is in the range of 65.2~ 126 $\mu mol \cdot g^{-1}$. The percentage of the sulfuric acid molecules related to the strong BA is 29.2 / (29.2 + 126) × 100% ~ 29.2 / (29.2 + 65.2) × 100% = 19 ~ 31 %

The density ratio of the newly generated LA to strong BA sites on T-SZ (3.5.2)

$D(LA) = S_{0\text{-}T} \times \text{Area percentage} \times X / (N_A \times U_{S\text{-}T(hkl)})$ (2)

According to the equation (2) in Section 3.5.2, for S-T(101), X = 0, D(LA) = 0 μmol·g^{-1}.

For S-T(001),

D(LA) = 40.4 m^2·g^{-1} × 4% × 4 / (6.022 × 10^{23} mol^{-1} × 52.6 Å^2) = 20.4 μmol·g^{-1}

For S-T(100),

D(LA) = 40.4 m^2·g^{-1} × 18% × 2 / (6.022 × 10^{23} mol^{-1} × 76.1 Å^2) = 31.7 μmol·g^{-1}

For structures on T(111), when S-T(111)-1 is the only structure on T(111),

D(LA) = 0 μmol·g^{-1} and the total LA density on T-SZ ($D(LA)_{total}$) is 20.4 + 31.7 = 52.1 μmol·g^{-1}.

When S-T(111)-2 is the only structure on T(111),

D(LA) = 40.4 m^2·g^{-1} × 17% × 2 / (6.022 × 10^{23} mol^{-1} ×59.8 Å^2) = 38.1 μmol·g^{-1} and $D(LA)_{total}$ = 20.4 + 31.7 + 38.1 = 90.2 μmol·g^{-1}.

When 2S-T(101) represents the structure on T(111),

D(LA) = 0 μmol·g^{-1} and $D(LA)_{total}$ = 20.4 + 31.7 + 0 = 52.1 μmol·g^{-1}

$D(BA) = S_{0\text{-}T} \times \text{area percentage} / (N_A \times U_{S\text{-}T(hkl)})$ (3)

According to equation (3) in Section 3.5.2, only structures on T(111) generate strong BA.

When S-T(111)-1 is the only structure on T(111),

D(BA) = 40.4 m^2·g^{-1} × 17% / (6.022 × 10^{23} mol^{-1} ×59.8 Å^2) = 19.1 μmol·g^{-1} and $D(LA)_{total}$:

D(BA) = 52.1 μmol·g^{-1} : 19.1 μmol·g^{-1} = 2.7:1.0.

When S-T(111)-2 is the only structure on T(111),

D(BA) = 40.4 m^2·g^{-1} × 17% / (6.022 × 10^{23} mol^{-1} ×59.8 Å^2) = 19.1 μmol·g^{-1} and $D(LA)_{total}$: D(BA) = 90.2 μmol·g^{-1} : 19.1 μmol·g^{-1} = 4.7:1.0.

When 2S-T(101) represents the structure on T(111),

D(BA) = 40.4 m^2·g^{-1} × 17% / (6.022 × 10^{23} mol^{-1} ×29.9 Å^2) = 38.1 μmol·g^{-1} and $D(LA)_{total}$: D(BA) = 52.1 μmol·g^{-1} : 38.1 μmol·g^{-1} = 1.4:1.0.

So the density ratio of the newly generated LA to strong BA sites is in the range of ca. 1.4:1.0 ~ 4.7:1.0.

The calculation detail of the optimized XYZ position for typical acid structures.

Optimized XYZ position for S-M(001)

Lengths	a	b	c	Angles	α	β	γ
Å	10.3746	10.5298	20.3527	degree	90	90	90

Atom	x	y	z
O	9.39879	1.02668	3.23194
O	4.21154	6.29152	3.23187
O	9.39912	6.29148	3.23207
O	1.33819	3.58505	3.6553
O	6.52507	3.58538	3.65535
O	1.3381	8.85002	3.65533
O	6.52516	8.85021	3.65537
Zr	2.98234	2.33424	4.1716
Zr	8.17007	2.33453	4.17143
Zr	2.98226	7.59939	4.17161
Zr	8.17025	7.59949	4.17136
Zr	0.1567	5.03383	4.45089
Zr	5.34452	5.03406	4.45094
Zr	0.15651	10.29883	4.45081
Zr	5.34445	10.29874	4.45096
O	1.73887	0.97484	4.8953
O	6.92553	0.97423	4.89541
O	1.73879	6.23957	4.89535
O	6.92543	6.23902	4.89543
O	3.72545	3.92097	5.39537
O	8.91268	3.92093	5.39541
O	3.72544	9.18587	5.39539
O	8.91267	9.18583	5.39543
O	4.12464	1.38091	5.83204
O	9.31196	1.38091	5.83218
O	4.12466	6.64578	5.83205
O	9.31196	6.64579	5.83221
O	0.84573	4.38801	6.46166
O	6.03294	4.38806	6.46154
O	0.84571	9.65292	6.46167
O	6.03296	9.65295	6.46158
Zr	2.6019	0.22651	6.7658
Zr	7.7892	0.22651	6.7658
Zr	2.6019	5.49141	6.7658
Zr	7.7892	5.49141	6.7658
Zr	4.83292	2.85897	7.20298
Zr	10.02022	2.85897	7.20298
Zr	4.83292	8.12387	7.20298
Zr	10.02022	8.12387	7.20298
O	1.41002	1.77661	7.46637
O	6.59732	1.77661	7.46637
O	1.41002	7.04151	7.46637
O	6.59732	7.04151	7.46637

O	3.24022	3.98873	8.20343
O	8.42752	3.98873	8.20343
O	3.24022	9.25363	8.20343
O	8.42752	9.25363	8.20343
O	3.7451	1.27621	8.40356
O	8.9324	1.27621	8.40356
O	3.7451	6.54111	8.40356
O	8.9324	6.54111	8.40356
O	0.388	3.48832	9.14062
O	5.5753	3.48832	9.14062
O	0.388	8.75322	9.14062
O	5.5753	8.75322	9.14062
Zr	2.1524	2.40597	9.40401
Zr	7.3397	2.40597	9.40401
Zr	2.1524	7.67087	9.40401
Zr	7.3397	7.67087	9.40401
Zr	4.38342	5.03843	9.8412
Zr	9.57072	5.03843	9.8412
Zr	4.38342	10.30333	9.8412
Zr	9.57072	10.30333	9.8412
O	0.9335	0.90118	10.15415
O	6.11984	0.87926	10.13091
O	0.95571	6.13394	10.15096
O	6.14026	6.16117	10.20711
O	2.90131	3.90193	10.79453
O	8.02372	3.90418	10.78489
O	2.79514	9.17739	10.78818
O	8.01504	9.1413	10.78817
O	3.27428	1.36722	11.23329
O	8.43655	1.32677	11.16421
O	3.25049	6.63301	11.13217
O	8.49223	6.59704	11.0793
O	0.02083	4.32724	11.73014
O	5.27244	4.33847	11.74636
O	0.00862	9.58672	11.75775
O	5.17107	9.54771	11.74746
Zr	1.61129	0.22617	12.13668
Zr	6.79968	0.18527	12.12939
Zr	1.63016	5.53924	12.12179
Zr	7.01673	5.42677	12.17056
Zr	4.11418	2.92206	12.49707
Zr	9.21981	2.85157	12.39001
Zr	3.82511	8.20901	12.44233
Zr	9.08397	8.13455	12.47538
O	0.5088	1.7337	13.01444
O	5.62195	1.64452	12.96046
O	0.48364	6.98513	12.87963
O	5.63945	7.03175	12.90425
O	2.2787	3.72419	13.32362
O	7.94108	3.97943	13.38766

O	2.67821	9.53509	13.4038
O	7.93021	9.58901	13.36331
O	8.05428	6.6604	13.71282
H	8.53645	6.029	14.27748
H	6.06205	7.25863	13.76191
O	4.61127	4.46085	14.37798
O	2.9713	6.48508	13.88895
S	3.96543	5.47278	15.22444
O	4.84298	6.51256	15.69185
O	2.8669	5.04997	16.04366
H	2.23205	6.88139	14.40903
H	1.56204	3.01525	13.32476

Optimized XYZ position for S-M(011)

Lengths	a	b	c	Angles	α	β	γ
Å	10.3746	7.5079	28.575	degree	90	90	83.1229

Atom	x	y	z
O	0.83105	6.40113	4.9427
O	6.01813	6.40143	4.94296
O	2.48057	1.71543	5.1065
O	7.66793	1.71519	5.106
Zr	3.82682	3.2554	5.50681
Zr	9.01368	3.25544	5.50661
O	3.33336	5.28935	5.26574
O	8.52073	5.2894	5.26576
Zr	4.34806	7.24231	5.59451
Zr	9.53483	7.24247	5.59429
O	4.70762	1.426	6.16596
O	9.89485	1.42625	6.16591
O	0.56997	3.75585	6.02391
O	5.75728	3.7558	6.0239
Zr	1.62817	5.50066	6.59217
Zr	6.81542	5.50084	6.59213
O	2.73507	7.36984	7.08388
O	7.92245	7.36991	7.08416
Zr	1.24775	1.96318	7.08875
Zr	6.43532	1.96312	7.089
O	2.82329	3.51747	7.22918
O	8.01061	3.51749	7.2291
O	10.28121	6.40457	7.38395
O	5.09368	6.40459	7.38397
O	10.41537	2.6227	8.68456
O	5.22798	2.62274	8.68468
O	2.3183	5.439	8.86132
O	7.50562	5.439	8.8614
Zr	3.87598	6.94746	8.99096
Zr	9.06322	6.94761	8.99077
O	2.36847	1.58747	9.01973
O	7.55579	1.58752	9.01989
Zr	3.45704	3.56223	9.30706
Zr	8.64436	3.56223	9.30706
O	4.64892	5.15305	9.9095
O	9.83623	5.15305	9.9095
O	4.77196	0.09338	9.93861
O	9.95928	0.09338	9.93861
Zr	0.77652	1.6842	10.54105
Zr	5.96383	1.6842	10.54105
O	1.86434	3.65202	10.81344
O	7.05166	3.65202	10.81344
Zr	1.22601	5.7311	10.86172
Zr	6.41333	5.7311	10.86172
O	2.81872	7.23729	10.9548

O	8.00604	7.23729	10.9548
O	4.19942	2.63515	11.12118
O	9.38673	2.63515	11.12118
O	10.40878	6.33007	12.45384
O	5.22146	6.33007	12.45384
O	1.41484	1.72794	12.62023
O	6.60215	1.72794	12.62023
Zr	3.00754	3.23412	12.71332
Zr	8.19486	3.23412	12.71332
O	2.36922	5.31321	12.76159
O	7.55654	5.31321	12.76159
Zr	3.45704	7.28103	13.03398
Zr	8.64436	7.28103	13.03398
O	3.74991	1.41798	13.63642
O	8.93723	1.41798	13.63642
O	4.77196	3.81218	13.66553
O	9.95927	3.81218	13.66553
Zr	0.77651	5.403	14.26797
Zr	5.96383	5.403	14.26797
O	1.86775	7.36792	14.55463
O	7.03764	7.36347	14.53945
Zr	0.35004	2.00342	14.59033
Zr	5.52274	1.99868	14.55724
O	1.90018	3.51532	14.71573
O	7.10912	3.54195	14.70847
O	4.21471	6.37077	14.89965
O	9.3925	6.36722	14.8584
O	4.23784	2.47457	16.13941
O	9.4722	2.48787	16.22687
O	1.39233	5.43706	16.39878
O	6.57451	5.4326	16.35602
Zr	2.97459	6.9233	16.52177
Zr	8.16752	7.00599	16.45419
O	1.47419	1.56304	16.49377
O	6.67704	1.62318	16.40814
Zr	2.54703	3.50814	16.96682
Zr	7.71811	3.49324	16.80817
O	3.77093	5.13663	17.46098
O	8.89042	5.13119	17.3469
O	3.70414	0.02914	17.64908
O	8.94057	0.09117	17.50529
Zr	10.32136	1.64082	17.96536
Zr	4.9942	1.72844	17.90411
O	0.83265	3.62415	18.28312
O	6.13602	3.59375	18.22995
Zr	10.65743	5.68881	18.23447
Zr	5.65517	5.71521	18.16507
O	1.74698	7.2253	18.42902
O	6.98626	7.31856	18.23951
O	3.3816	2.62635	18.61093

O	8.5721	2.55716	18.76959
H	7.9645	1.92423	19.19987
H	7.24395	4.37118	20.14237
S	8.3402	6.1413	20.95061
O	9.55626	5.87399	20.10126
O	7.07336	5.33933	20.08677
O	7.93645	7.51868	20.91998
O	8.39805	5.42557	22.18976

Optimized XYZ position for S-T(111)-1

Lengths	a	b	c	Angles	α	β	γ
Å	10.2592	6.3733	27.6706	degree	90	90	66.2762

Atom	x	y	z
O	3.51158	2.19731	6.33699
O	8.64118	2.19731	6.33699
Zr	4.66312	3.7109	7.1297
Zr	9.79272	3.7109	7.1297
O	3.71395	5.54856	7.30903
O	8.84355	5.54856	7.30903
O	6.18734	5.20706	7.56457
O	11.31694	5.20706	7.56457
Zr	2.58219	1.23317	7.88118
Zr	7.71179	1.23317	7.88118
O	3.50199	3.24628	8.68191
O	8.63159	3.24628	8.68191
O	6.01755	2.61725	8.3085
O	11.14715	2.61725	8.3085
Zr	2.46454	5.03609	9.07933
Zr	7.59414	5.03609	9.07933
O	3.80856	0.94265	9.6003
O	8.93816	0.94265	9.6003
O	1.25681	0.57227	9.84712
O	6.38641	0.57227	9.84712
Zr	5.13075	2.45192	10.29317
Zr	10.26035	2.45192	10.29317
O	6.41286	4.41661	10.75941
O	11.54246	4.41661	10.75941
O	3.84805	3.96931	10.97838
O	8.97765	3.96931	10.97838
Zr	2.566	0.09922	11.44465
Zr	7.6956	0.09922	11.44465
O	1.28332	2.06329	11.91117
O	6.41292	2.06329	11.91117
O	3.84808	1.61529	12.13037
O	8.97768	1.61529	12.13037
Zr	2.56536	3.57939	12.59689
Zr	7.69496	3.57939	12.59689
O	3.84748	5.54408	13.06313
O	8.97708	5.54408	13.06313
O	6.41226	5.09675	13.28211
O	11.54186	5.09675	13.28211
Zr	5.1302	1.22665	13.74837
Zr	10.2598	1.22665	13.74837
O	3.85578	3.13191	14.20806
O	8.98641	3.12502	14.20247
O	1.30089	2.75206	14.37398
O	6.43303	2.76077	14.39452
Zr	5.17078	4.58484	14.9749

Zr	10.3071	4.58219	14.93739
O	4.20626	1.02924	15.68442
O	9.30736	1.01033	15.66616
O	1.60555	0.48291	15.49008
O	6.68933	0.47014	15.46591
Zr	2.58829	2.4708	15.99798
Zr	7.73945	2.48848	15.99817
O	3.94247	3.95414	16.70576
O	9.09269	3.95599	16.68385
O	6.61939	4.29603	16.43793
O	11.73079	4.27599	16.38272
Zr	2.83931	5.70696	17.04524
Zr	8.02567	5.72794	17.0277
O	1.52609	1.66041	17.67378
O	6.8923	1.54275	17.7105
H	11.67579	2.14724	18.50833
O	12.42336	5.71334	18.94002
H	12.75018	6.04794	19.78917
O	18.75915	5.0173	19.27663
S	17.79918	6.24092	20.01126
O	18.75089	7.23984	20.44314
O	17.0946	6.58582	18.72385
O	16.96018	5.60833	20.97927
H	19.67944	5.06467	19.61345
H	19.62712	7.73208	18.62089

Optimized XYZ position for S-T(111)-2

Lengths	a	b	c	Angles	α	β	γ
Å	10.2592	6.3733	27.6706	degree	90	90	66.2762

Atom	x	y	z
O	3.51158	2.19731	6.33699
O	8.64118	2.19731	6.33699
Zr	4.66312	3.7109	7.1297
Zr	9.79272	3.7109	7.1297
O	3.71395	5.54856	7.30903
O	8.84355	5.54856	7.30903
O	6.18734	5.20706	7.56457
O	11.31694	5.20706	7.56457
Zr	2.58219	1.23317	7.88118
Zr	7.71179	1.23317	7.88118
O	3.50199	3.24628	8.68191
O	8.63159	3.24628	8.68191
O	6.01755	2.61725	8.3085
O	11.14715	2.61725	8.3085
Zr	2.46454	5.03609	9.07933
Zr	7.59414	5.03609	9.07933
O	3.80856	0.94265	9.6003
O	8.93816	0.94265	9.6003
O	1.25681	0.57227	9.84712
O	6.38641	0.57227	9.84712
Zr	5.13075	2.45192	10.29317
Zr	10.26035	2.45192	10.29317
O	6.41286	4.41661	10.75941
O	11.54246	4.41661	10.75941
O	3.84805	3.96931	10.97838
O	8.97765	3.96931	10.97838
Zr	2.566	0.09922	11.44465
Zr	7.6956	0.09922	11.44465
O	1.28332	2.06329	11.91117
O	6.41292	2.06329	11.91117
O	3.84808	1.61529	12.13037
O	8.97768	1.61529	12.13037
Zr	2.56536	3.57939	12.59689
Zr	7.69496	3.57939	12.59689
O	3.84748	5.54408	13.06313
O	8.97708	5.54408	13.06313
O	6.41226	5.09675	13.28211
O	11.54186	5.09675	13.28211
Zr	5.1302	1.22665	13.74837
Zr	10.2598	1.22665	13.74837
O	3.85647	3.12388	14.21215
O	9.01055	3.13096	14.20255
O	1.323	2.73453	14.4183
O	6.45346	2.74076	14.42192
Zr	5.26875	4.49254	14.96545

Zr	10.2998	4.5638	14.95206
O	4.22092	1.04241	15.66386
O	9.35518	1.01537	15.68269
O	1.6878	0.42169	15.52575
O	6.67408	0.44267	15.37289
Zr	2.60726	2.46267	16.02179
Zr	7.70408	2.4408	16.14696
O	3.98236	3.89292	16.70372
O	9.11859	4.0045	16.77827
O	6.65096	4.28834	16.45078
O	11.79549	4.34313	16.4319
Zr	2.97919	5.72412	16.97003
Zr	8.0862	5.83711	17.0216
O	1.15433	1.88519	17.55459
O	6.8418	1.4715	17.68043
O	4.27326	5.33692	18.87752
S	5.63574	6.15396	19.61513
O	5.02551	7.26471	20.27401
O	6.25513	5.08298	20.34546
O	6.44572	6.56953	18.41209
H	3.18699	8.48239	17.85281
H	4.57183	4.40463	18.75497

Optimized XYZ position for 2S-T(111)

Lengths	a	b	c	Angles	α	β	γ
Å	10.2592	6.3733	27.6706	degree	90	90	66.2762

Atom	x	y	z
O	3.51158	2.19731	6.33699
O	8.64118	2.19731	6.33699
Zr	4.66312	3.7109	7.1297
Zr	9.79272	3.7109	7.1297
O	3.71395	5.54856	7.30903
O	8.84355	5.54856	7.30903
O	6.18734	5.20706	7.56457
O	11.31694	5.20706	7.56457
Zr	2.58219	1.23317	7.88118
Zr	7.71179	1.23317	7.88118
O	3.50199	3.24628	8.68191
O	8.63159	3.24628	8.68191
O	6.01755	2.61725	8.3085
O	11.14715	2.61725	8.3085
Zr	2.46454	5.03609	9.07933
Zr	7.59414	5.03609	9.07933
O	3.80856	0.94265	9.6003
O	8.93816	0.94265	9.6003
O	1.25681	0.57227	9.84712
O	6.38641	0.57227	9.84712
Zr	5.13075	2.45192	10.29317
Zr	10.26035	2.45192	10.29317
O	6.41286	4.41661	10.75941
O	11.54246	4.41661	10.75941
O	3.84805	3.96931	10.97838
O	8.97765	3.96931	10.97838
Zr	2.566	0.09922	11.44465
Zr	7.6956	0.09922	11.44465
O	1.28332	2.06329	11.91117
O	6.41292	2.06329	11.91117
O	3.84808	1.61529	12.13037
O	8.97768	1.61529	12.13037
Zr	2.56536	3.57939	12.59689
Zr	7.69496	3.57939	12.59689
O	3.84748	5.54408	13.06313
O	8.97708	5.54408	13.06313
O	6.41226	5.09675	13.28211
O	11.54186	5.09675	13.28211
Zr	5.1302	1.22665	13.74837
Zr	10.2598	1.22665	13.74837
O	3.89294	3.11551	14.19106
O	9.02053	3.11206	14.18759
O	1.35062	2.71911	14.39467
O	6.47785	2.71824	14.3959
Zr	5.23316	4.54021	14.96146

Zr	10.36429	4.52963	14.96169
O	4.25798	0.99895	15.68751
O	9.38996	1.00895	15.69475
O	1.65302	0.42114	15.51507
O	6.80414	0.41941	15.53762
Zr	2.65599	2.42594	16.00606
Zr	7.77604	2.42501	16.00428
O	4.03499	3.88513	16.68342
O	9.16103	3.87731	16.67249
O	6.69813	4.27943	16.40675
O	11.82491	4.26839	16.40987
Zr	2.97778	5.64317	17.05995
Zr	8.11444	5.63513	17.06887
O	1.60838	1.64046	17.68615
O	6.61548	1.71327	17.652
H	8.38213	11.66579	19.14908
H	3.17052	11.75926	19.04011
O	9.30706	11.9137	18.91719
O	4.07283	12.1067	18.81972
O	11.47794	10.99789	19.10273
O	6.15887	11.00309	19.13949
O	9.82506	10.30655	20.8104
O	4.51339	10.8711	20.98969
O	10.80906	12.60186	20.83992
O	5.72056	12.99992	20.48698
S	10.44084	11.40993	20.1392
S	5.19542	11.72695	20.07446
H	8.97371	8.04144	18.46818
H	14.27796	7.85903	18.57485

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