Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First-Principles Study of CO_2 hydrogenation to formic acid on single-atom catalysts supported on SiO_2

Jikai Sun[a], Shuchao Jiang[a], Yanliang Zhao[a], Honglei Wang[a], Dong Zhai[a], Weiqiao Deng[,a,b], and Lei Sun[*,a]*

[a]Institute of Molecular Sciences and Engineering, Institute of Frontier and Interdisciplinary Science, Shandong University, Qingdao 266237, R. P. China. E-mail: slei@sdu.edu.cn & dengwq@sdu.edu.cn

[b]State Key Laboratory of Molecular Reaction Dynamics, Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, R. P. China

Table S1 Energy difference of different convergence criteria. $\Delta E = E(0.01) - E(0.02)$

Model	ΔE (kcal/mol)
Pt@SiO_2	-0.0004612
Ir@SiO_2-CO_2	-0.0002306
Au@SiO_2-H_2	-0.005765
Rh@SiO_2-H_2	-0.0004612
Ru@SiO_2-H_2	-0.3601972
Ru@SiO_2-2H	-0.0163726
Os@SiO_2-H-CO_2	-0.0108382
Pd@SiO_2-H-CO_2	-0.0445058
Ru@SiO_2-H-CO_2	-0.0915482
Ru@SiO_2-OCHO-TS	-0.1219874
Ru@SiO_2-OCHO	-0.0285944

Table S2 Ideal value of <S**2>. $< S ** 2 > = S \times (S + 1)$, where S denoted spin quantum number.

	$M@SiO_2$	$M@SiO_2$-CO_2	$M@SiO_2$-H_2	$M@SiO_2$-H	$M@SiO_2$-H-CO_2
Ru	3.75	3.75	3.75	2.00	2.00
Rh	0.00	0.00	2.00	0.75	0.75
Pd	0.75	0.75	0.75	2.00	0.00
Ag	2.00	-	2.00	-	-
Os	3.75	0.75	0.75	2.00	2.00
Ir	2.00	2.00	2.00	3.75	0.75
Pt	0.75	0.75	0.75	2.00	0.00
Au	2.00	0.00	0.00	0.75	0.75

The '-' sign denoted not calculated.

Table S3 Surface energy (E_{surf}) of diffenent surface of β-cristobalite.

Surface	E_{surf} (J/m^2)
100	2.77
101	2.13
110	2.35
111	1.97

Table S4 Energy of H_2 adsorption and dissociation (unit: kcal/mol).

Metal	E_{ad}	Barrier	E_r
Rh	-18.79	28.43	-3.79
Pd	-14.82	13.19	-21.37
Pt	-25.1	18.45	-13.48
Au	-20.31	10.44	-38.82

Table S5 Energy of CO_2 hydrogenation (unit: kcal/mol).

Metal	Barrier	E_r
Ru	23.93	6.42
Rh	31.54	14.16
Pd	31.91	14.25
Os	24.93	-2.81
Ir	30.17	2.66
Pt	31.93	8.13
Au	56.95	23.28

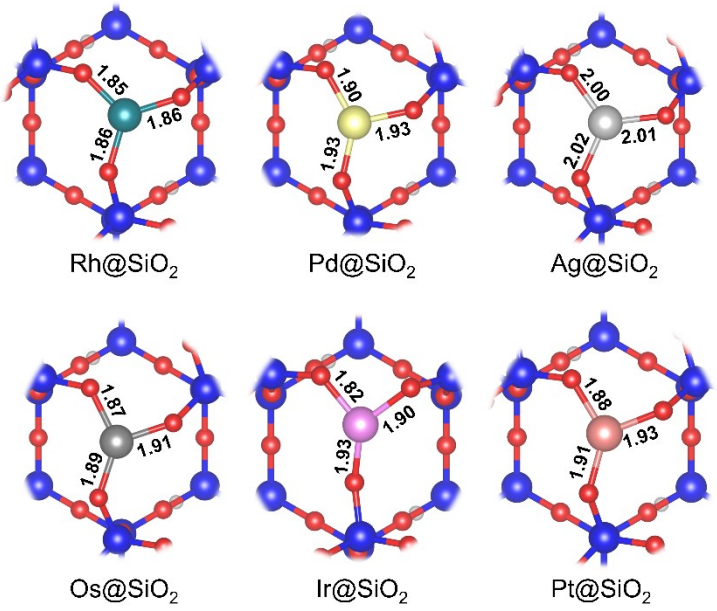

Figure S1 Optimized structure of singly dispersed metal atoms anchored on inert support SiO_2**.**

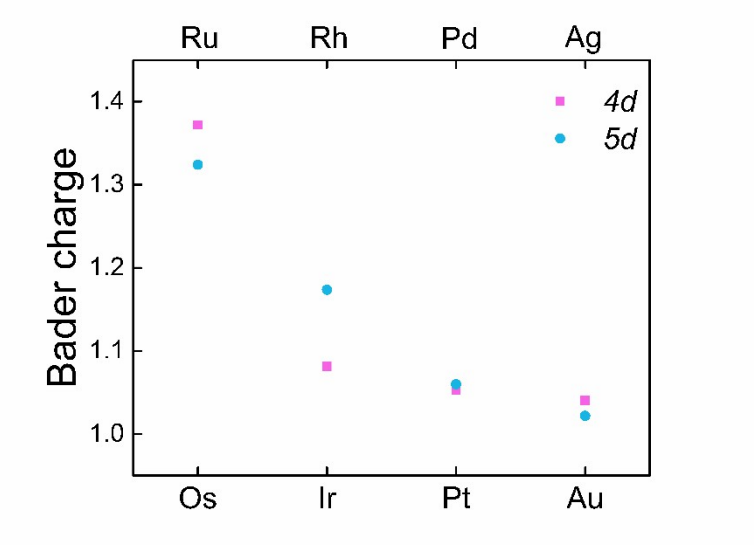

Figure S2 Bader charge of eight noble metals of M@SiO_2.

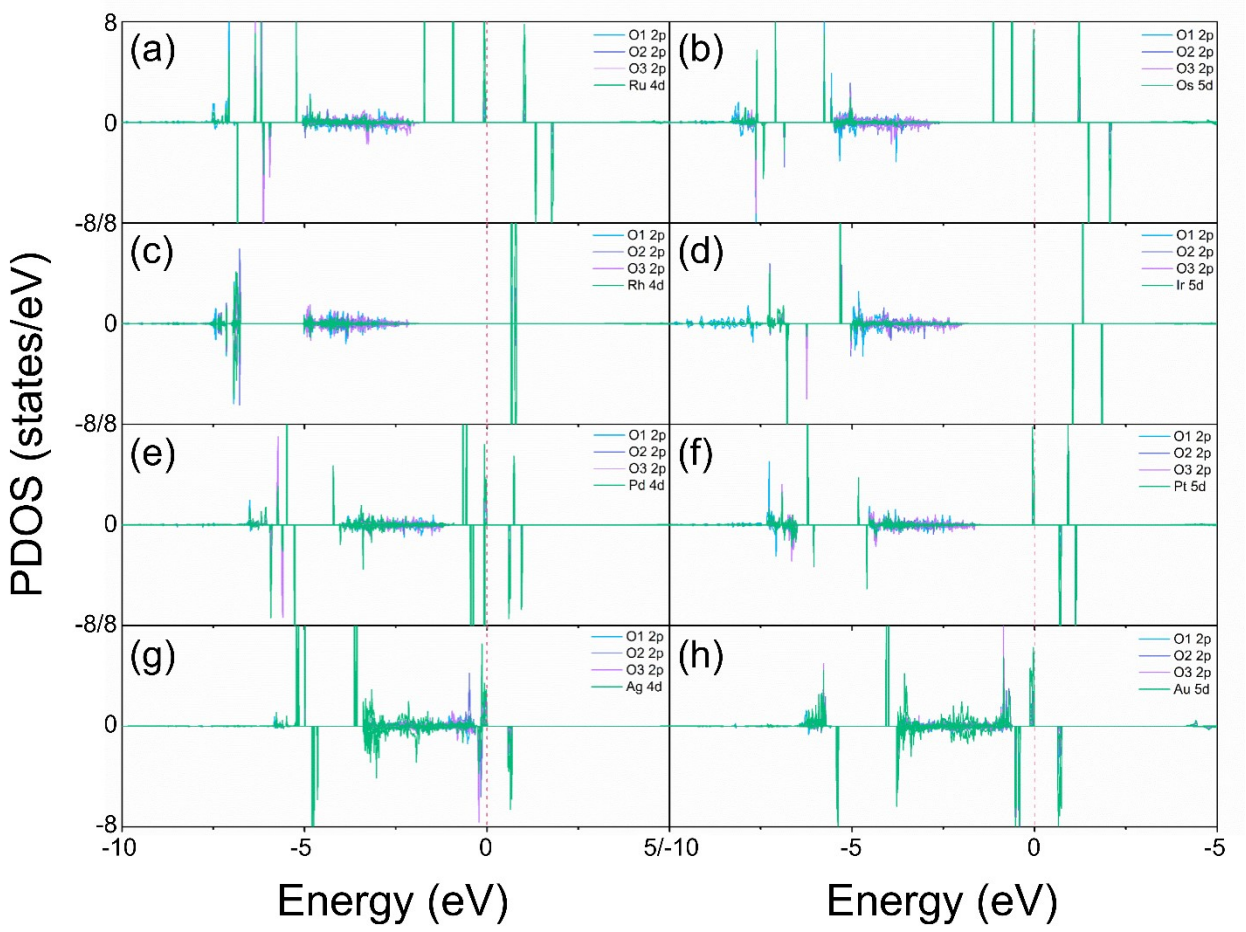

Figure S3 PDOS of p-orbitals of metal-coordinated oxygen and d-orbitals of the metal atom of eight M@SiO_2. The Fermi level is set to zero.

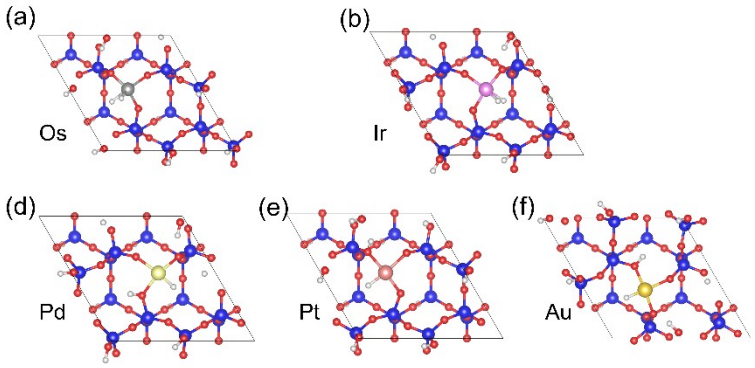

Figure S4 Optimized structure of two hydrogen atoms adsorbed on M@SiO_2.

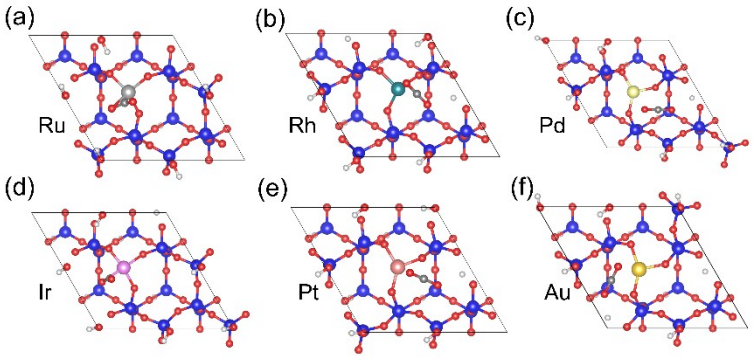

Figure S5 Optimized structure of CO_2 molecule adsorbed on M@SiO_2.

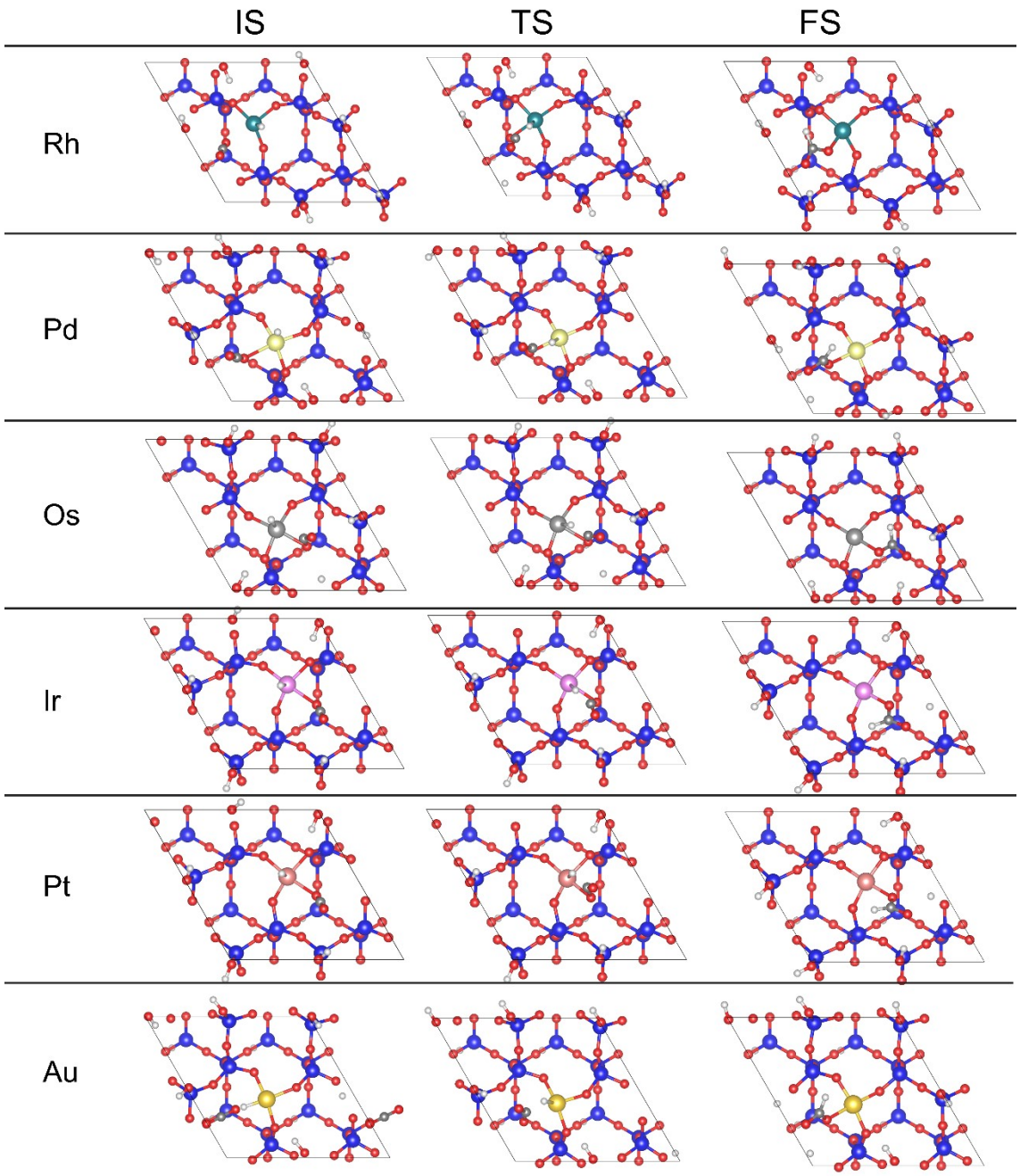

Figure S6 Structure of CO_2 hydrogenation to formate, including initial state (IS), transition state (TS), and final state (FS).

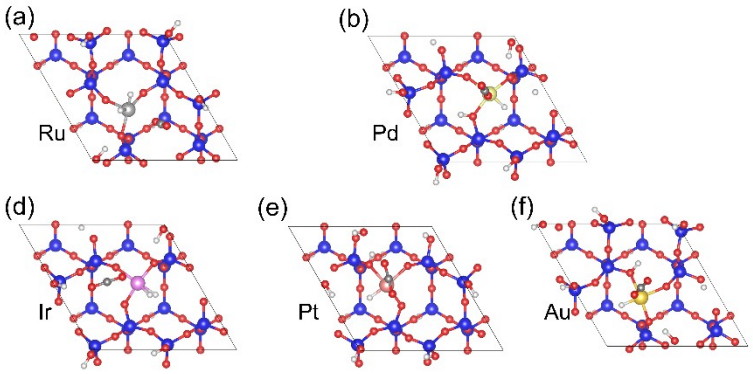

Figure S7 Optimized structure of CO_2 molecule adsorbed on M@SiO_2-2H.

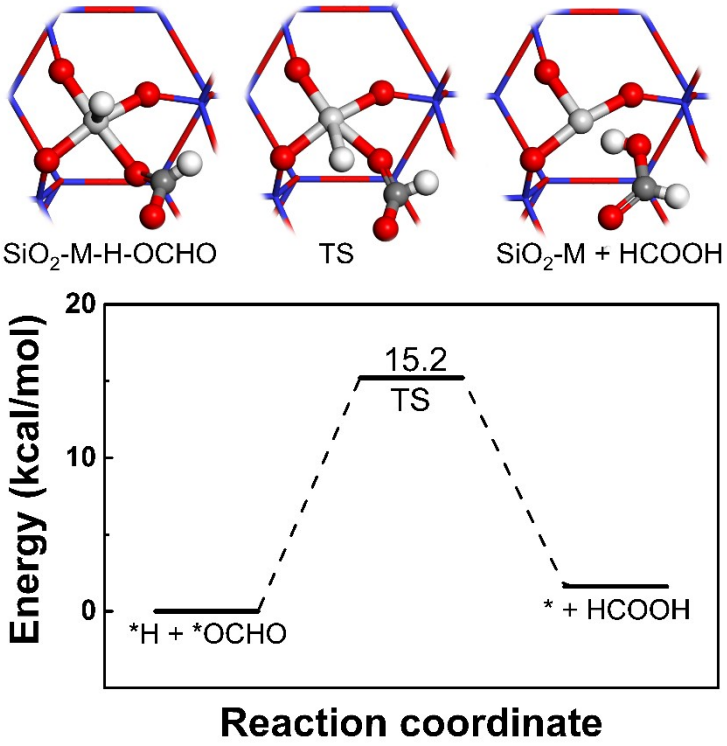

Figure S8 Energy profile of *HCOO hydrogenation to formic acid on Ru@SiO_2 and corresponding structures, including initial state (IS), transition state (TS), and final state (FS).

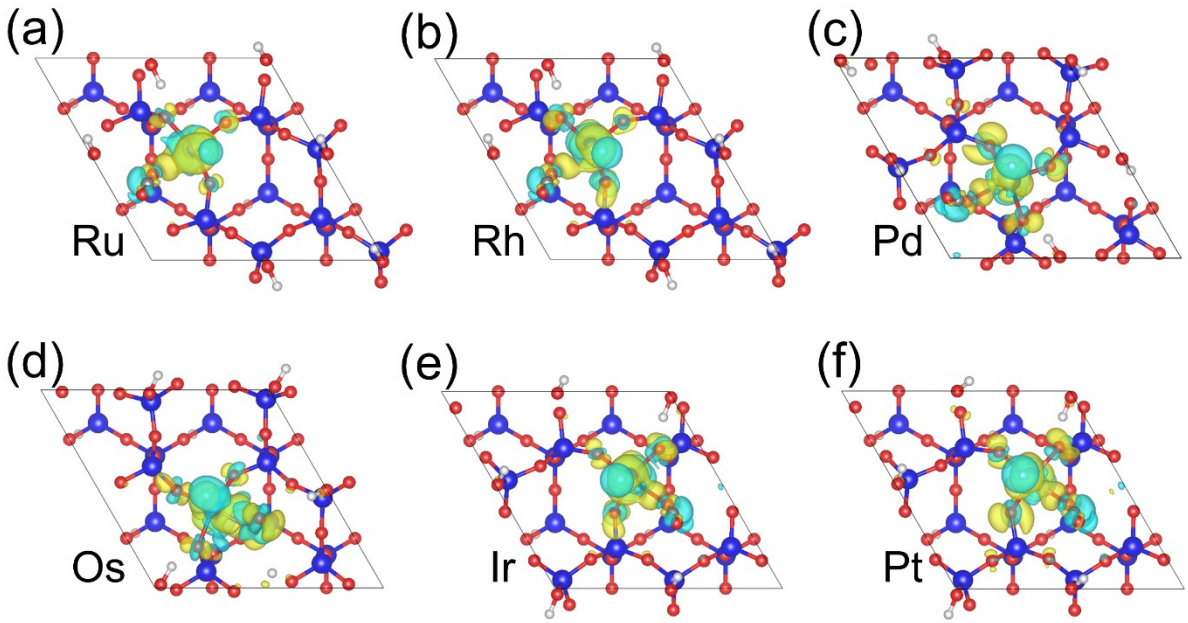

Figure S9 Charge density difference between H and CO_2 and Ru@SiO_2 (a), Rh@SiO_2 (b), Pd@SiO_2 (c), Os@SiO_2 (d), Ir@SiO_2 (e), and Pt@SiO_2 (f), respectively. The charge density difference was calculated by the pattern of Charge(M@SiO_2-H-CO_2) – Charge(M@SiO_2) – Charge(H and CO_2). Isosurface level is 0.0025 e $Bohr^{-3}$. The yellow and green colors represent electron accumulation and depletion, respectively.

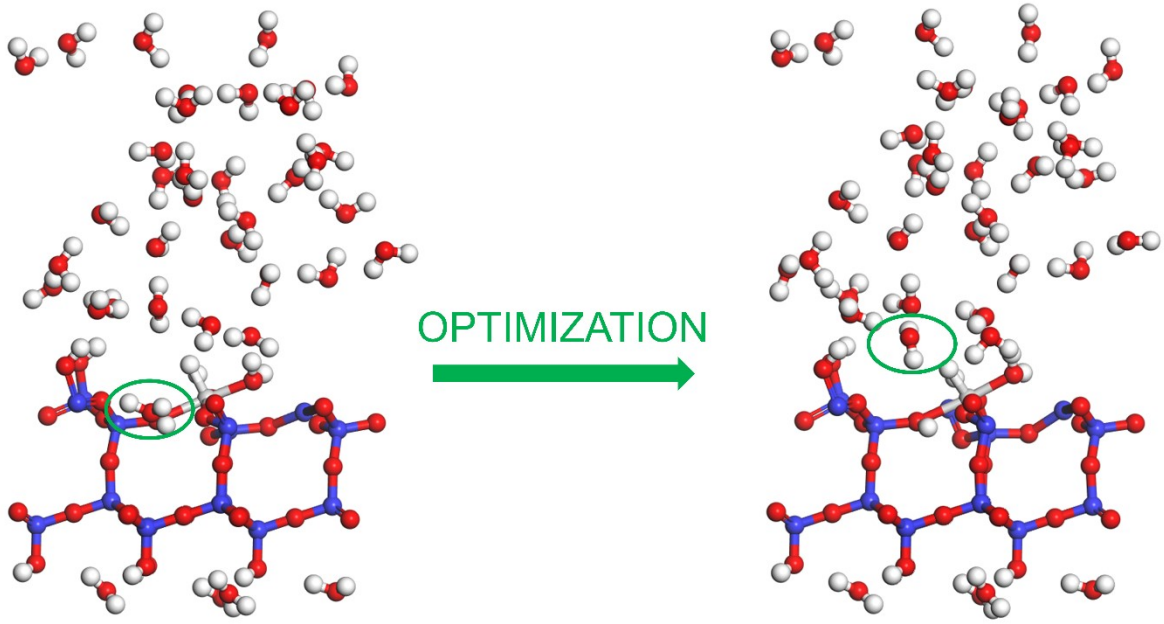

Figure S10 Water adsorption configurations before and after optimization.

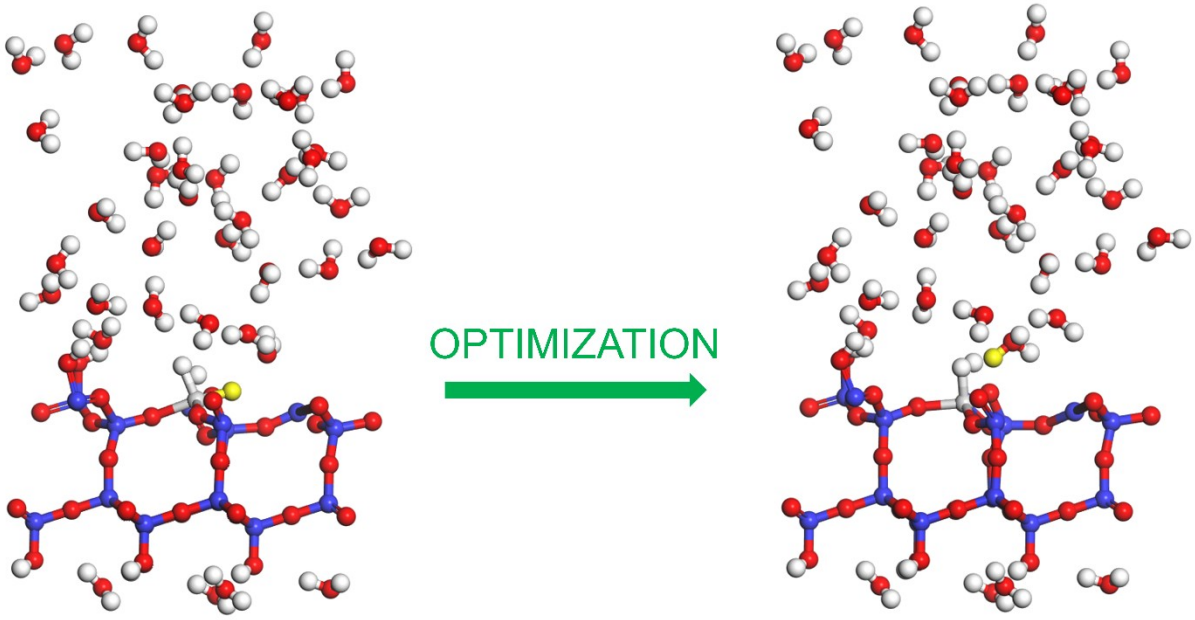

Figure S11 Configurations of Ru@SiO_2-2H before and after optimization.

Coordinates:

73

Ru@SiO2

Si	5.291085	9.062113	9.287902
Si	2.637872	1.523037	5.062270
Si	2.546461	1.440962	8.287803
Si	0.000053	3.045983	3.985274
Si	5.298813	0.325028	9.238218
Si	7.913722	1.523037	5.062270
Si	8.053050	1.715833	8.271247
Si	5.275903	3.045983	3.985274
Si	-2.448154	4.797381	9.281199
Si	-0.000053	6.092057	5.062270
Si	0.021881	6.578857	8.211360
Si	-2.637872	7.615002	3.985274
Si	5.275797	6.092057	5.062270
Si	5.289093	6.048809	8.294136
Si	2.637978	7.615002	3.985274
O	0.179705	0.034230	10.915421
O	2.671002	1.534867	6.678614
O	0.000053	3.045983	2.370024
O	2.637925	0.000000	4.523772
O	-2.637925	9.138040	4.523772
O	1.952375	2.831460	8.906308
O	4.020713	1.293509	8.953711
O	1.318962	2.284510	4.523772
O	-1.318962	2.284510	4.523772

O	9.232738	2.284510	4.523772
O	1.491228	0.267508	8.672683
O	0.120176	9.040304	10.818191
O	7.919852	1.521648	6.674094
O	5.275903	3.045983	2.370024
O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	8.186584	3.307249	8.606687
O	9.388925	0.939786	8.784210
O	6.594812	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.704719	1.086308	8.944979
O	-2.494941	4.686852	10.917069
O	0.021659	6.054574	6.678068
O	-2.637872	7.615002	2.370024
O	0.000000	4.569020	4.523772
O	-0.284309	8.173724	8.266099
O	1.525939	6.430648	8.872843
O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772
O	6.594812	6.853530	4.523772
O	-1.086069	5.659919	8.988136
O	5.223598	6.065162	6.672819
O	2.637978	7.615002	2.370024
O	5.275849	4.569020	4.523772
O	4.942895	7.553484	8.811562
O	6.805634	5.594942	8.706984

O 3.956887 6.853530 4.523772

O 1.318963 6.853530 4.523772

O 4.232547 5.017694 8.985062

Ru 2.309101 4.679344 8.865439

H 9.920052 0.031823 11.445251

H -0.906338 2.522739 2.000066

H -0.668814 8.644214 11.220270

H 4.369512 2.522739 2.000066

H 7.258019 4.299435 11.306645

H -3.544263 7.091758 2.000066

H 1.731587 7.091758 2.000066

O 4.113075 10.077826 8.784210

O 6.767077 9.405547 8.672683

O 5.455554 9.172270 10.915421

O 4.991540 -0.964315 8.266099

O 5.396026 -0.097735 10.818191

O -2.365116 3.307249 8.606687

O -3.746066 5.594942 8.706984

H -0.631648 0.031823 11.445251

H -3.293680 4.299435 11.306645

H 4.644202 9.169863 11.445251

H 4.607036 -0.493826 11.220270

74

Ru@SiO2-H2

Si 5.272873 9.003213 9.274261

Si 2.637872 1.523037 5.062270

Si	2.509106	1.427073	8.282057
Si	0.000053	3.045983	3.985274
Si	5.241642	0.293340	9.207611
Si	7.913722	1.523037	5.062270
Si	8.022676	1.663419	8.275829
Si	5.275903	3.045983	3.985274
Si	-2.604173	4.743137	9.283559
Si	-0.000053	6.092057	5.062270
Si	-0.141737	6.583446	8.192525
Si	-2.637872	7.615002	3.985274
Si	5.275797	6.092057	5.062270
Si	5.103673	5.968779	8.282769
Si	2.637978	7.615002	3.985274
O	0.205049	0.030438	10.896035
O	2.675537	1.527555	6.678923
O	0.000053	3.045983	2.370024
O	2.637925	0.000000	4.523772
O	-2.637925	9.138040	4.523772
O	1.884921	2.784341	8.912205
O	3.966988	1.281204	8.993694
O	1.318962	2.284510	4.523772
O	-1.318962	2.284510	4.523772
O	9.232738	2.284510	4.523772
O	1.449656	0.222565	8.611572
O	0.078510	8.951926	10.773777
O	7.916806	1.521576	6.674175
O	5.275903	3.045983	2.370024

O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	8.168946	3.244639	8.661989
O	9.342434	0.857805	8.785040
O	6.594812	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.656981	1.038746	8.917974
O	-2.456417	4.686024	10.921931
O	0.025700	6.034534	6.679958
O	-2.637872	7.615002	2.370024
O	0.000000	4.569020	4.523772
O	-0.376454	8.192996	8.181753
O	1.259764	6.404540	9.037960
O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772
O	6.594812	6.853530	4.523772
O	-1.398086	5.754555	8.838947
O	5.266628	6.092134	6.675566
O	2.637978	7.615002	2.370024
O	5.275849	4.569020	4.523772
O	4.896570	7.470344	8.888956
O	6.493901	5.317676	8.854476
O	3.956887	6.853530	4.523772
O	1.318963	6.853530	4.523772
O	3.848444	5.023310	8.704341
Ru	2.011267	4.646044	9.246872
H	4.688926	9.074534	11.446683

H -0.906338 2.522739 2.000066

H -0.726904 8.587405 11.173402

H 4.369512 2.522739 2.000066

H 7.416548 4.187681 11.402337

H -3.544263 7.091758 2.000066

H 1.731587 7.091758 2.000066

H 0.881316 4.367198 10.591825

H 0.365479 4.288532 9.925492

O 4.066584 9.995844 8.785040

O 6.725506 9.360605 8.611572

O 5.480899 9.168478 10.896035

O 4.899395 -0.945044 8.181753

O 5.354360 -0.186113 10.773777

O -2.382753 3.244639 8.661989

O -4.057798 5.317676 8.854476

H -0.586924 -0.063505 11.446683

H -3.135152 4.187681 11.402337

H 4.548945 -0.550634 11.173402

74

Ru@SiO2-H2-TS

Si 5.114773 9.030598 9.273360

Si 2.637872 1.523037 5.062270

Si 2.368803 1.443678 8.261452

Si 0.000053 3.045983 3.985274

Si 5.095818 0.325932 9.186426

Si 7.913722 1.523037 5.062270

Si	7.884201	1.706783	8.274128
Si	5.275903	3.045983	3.985274
Si	-2.735012	4.786014	9.272099
Si	-0.000053	6.092057	5.062270
Si	-0.290319	6.620057	8.170047
Si	-2.637872	7.615002	3.985274
Si	5.275797	6.092057	5.062270
Si	4.995225	6.001855	8.262498
Si	2.637978	7.615002	3.985274
O	0.143755	0.002285	10.884528
O	2.675236	1.510402	6.678549
O	0.000053	3.045983	2.370024
O	2.637925	0.000000	4.523772
O	-2.637925	9.138040	4.523772
O	1.731208	2.847671	8.778846
O	3.762837	1.260115	9.083447
O	1.318962	2.284510	4.523772
O	-1.318962	2.284510	4.523772
O	9.232738	2.284510	4.523772
O	1.246862	0.290792	8.538980
O	0.033325	8.962936	10.733565
O	7.921147	1.514295	6.673834
O	5.275903	3.045983	2.370024
O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	8.010244	3.295812	8.622378
O	9.142542	0.887950	8.908075

O	6.594812	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.457920	1.132632	8.825305
O	-2.467075	4.733316	10.893981
O	0.020109	6.048291	6.684160
O	-2.637872	7.615002	2.370024
O	0.000000	4.569020	4.523772
O	-0.503640	8.233455	8.141680
O	1.062151	6.420212	9.094213
O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772
O	6.594812	6.853530	4.523772
O	-1.602102	5.826976	8.721845
O	5.314852	6.112223	6.674615
O	2.637978	7.615002	2.370024
O	5.275849	4.569020	4.523772
O	4.741014	7.508153	8.846936
O	6.317703	5.337441	8.968858
O	3.956887	6.853530	4.523772
O	1.318963	6.853530	4.523772
O	3.672500	5.090643	8.499755
Ru	1.851322	4.678478	9.211596
H	4.651963	9.099406	11.475194
H	-0.906338	2.522739	2.000066
H	-0.730806	8.554250	11.170488
H	4.369512	2.522739	2.000066
H	7.450778	4.225708	11.424039

H -3.544263 7.091758 2.000066

H 1.731587 7.091758 2.000066

H 1.870388 4.539341 10.802530

H 0.691870 4.377813 10.340631

O 3.866692 10.025990 8.908075

O 6.522712 9.428831 8.538980

O 5.419605 9.140325 10.884528

O 4.772210 -0.904585 8.141680

O 5.309175 -0.175103 10.733565

O -2.541455 3.295812 8.622378

O -4.233996 5.337441 8.968858

H -0.623887 -0.038633 11.475194

H -3.100921 4.225708 11.424039

H 4.545043 -0.583790 11.170488

73

Ru@SiO2-CO2

Si -0.232767 0.413575 9.215633

Si 2.637872 1.523037 5.062270

Si 2.474390 1.799931 8.240976

Si 0.000053 3.045983 3.985274

Si 5.012016 0.306949 9.103045

Si 7.913722 1.523037 5.062270

Si 7.666073 1.906839 8.230589

Si 5.275903 3.045983 3.985274

Si 7.573821 4.986397 9.170162

Si -0.000053 6.092057 5.062270

Si	-0.469347	6.651497	8.096396
Si	-2.637872	7.615002	3.985274
Si	5.275797	6.092057	5.062270
Si	4.991982	6.514604	8.220888
Si	2.637978	7.615002	3.985274
O	-0.014860	0.039832	10.793795
O	2.683715	1.453537	6.677736
O	0.000053	3.045983	2.370024
O	2.637925	0.000000	4.523772
O	-2.637925	9.138040	4.523772
O	2.799544	3.401776	8.427488
O	3.580158	1.079923	9.187808
O	1.318962	2.284510	4.523772
O	-1.318962	2.284510	4.523772
O	9.232738	2.284510	4.523772
O	0.956716	1.394014	8.658379
O	0.032157	8.798162	10.572720
O	7.920507	1.544620	6.674554
O	5.275903	3.045983	2.370024
O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	7.666142	3.530219	8.434644
O	8.887527	1.190961	9.048852
O	6.594812	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.208288	1.327570	8.669521
O	-2.592116	4.723816	10.737873

O	0.039788	6.012231	6.689820
O	-2.637872	7.615002	2.370024
O	0.000000	4.569020	4.523772
O	-0.477918	8.275064	7.959008
O	0.637850	6.323750	9.279133
O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772
O	6.594812	6.853530	4.523772
O	-1.928961	6.027800	8.453230
O	5.261426	6.106641	6.678319
O	2.637978	7.615002	2.370024
O	5.275849	4.569020	4.523772
O	5.135017	8.132471	8.405876
O	6.087996	5.678209	9.098056
O	3.956887	6.853530	4.523772
O	1.318963	6.853530	4.523772
O	3.450966	6.130671	8.647627
O	0.792204	3.780343	10.408113
O	2.335324	4.263713	12.130549
Ru	2.010918	4.977262	9.109155
H	-0.297237	0.695567	11.449759
H	-0.906338	2.522739	2.000066
H	0.464256	7.922637	10.541378
H	4.369512	2.522739	2.000066
H	-2.886229	5.385186	11.383039
H	-3.544263	7.091758	2.000066
H	1.731587	7.091758	2.000066

C 1.748210 4.192377 11.099545

O -0.140833 -1.005569 8.405876

O -1.664173 1.190961 9.048852

O 4.797932 -0.862976 7.959008

O 5.308007 -0.339877 10.572720

O 8.622739 6.027800 8.453230

O 7.959583 4.723816 10.737873

H 5.740106 -1.215402 10.541378

H 7.665470 5.385186 11.383039

76

Ru@SiO2-H-CO2

Si 10.305301 0.372783 9.188687

Si 2.637872 1.523037 5.062270

Si 2.451345 1.847490 8.233866

Si 0.000053 3.045983 3.985274

Si 4.989909 0.369129 9.082150

Si 7.913722 1.523037 5.062270

Si 7.677102 1.935262 8.223415

Si 5.275903 3.045983 3.985274

Si 7.522222 5.043006 9.115244

Si -0.000053 6.092057 5.062270

Si -0.521560 6.736414 8.075017

Si -2.637872 7.615002 3.985274

Si 5.275797 6.092057 5.062270

Si 4.917120 6.516054 8.184742

Si 2.637979 7.615002 3.985274

O	5.193173	9.065343	10.758425
O	2.654365	1.453928	6.680225
O	0.000053	3.045983	2.370024
O	2.637925	0.000000	4.523772
O	-2.637925	9.138040	4.523772
O	2.652770	3.466136	8.363524
O	3.610807	1.224378	9.184717
O	1.318963	2.284510	4.523772
O	-1.318962	2.284510	4.523772
O	9.232738	2.284510	4.523772
O	0.980539	1.357519	8.731531
O	-0.012074	8.834348	10.545048
O	7.938760	1.557562	6.675110
O	5.275903	3.045983	2.370024
O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	7.656182	3.562967	8.427085
O	8.915032	1.248232	9.056538
O	6.594811	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.232566	1.340112	8.664576
O	-2.592505	4.804316	10.687956
O	0.035849	6.052324	6.698512
O	-2.637872	7.615002	2.370024
O	0.000000	4.569019	4.523772
O	-0.567506	8.360520	7.922078
O	0.590760	6.474653	9.270148

O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772
O	6.594812	6.853530	4.523772
O	-1.986546	6.090904	8.399217
O	5.300383	6.078029	6.670308
O	2.637979	7.615002	2.370024
O	5.275849	4.569019	4.523772
O	5.117420	8.145391	8.313023
O	6.021626	5.692573	9.095911
O	3.956887	6.853530	4.523772
O	1.318963	6.853530	4.523772
O	3.362917	6.234150	8.512498
O	0.060161	3.866733	9.675701
O	-0.409714	2.965986	11.794251
Ru	1.898643	5.071154	8.994569
H	10.104123	0.514950	11.437623
H	-0.906338	2.522739	2.000066
H	0.412511	7.952667	10.467817
H	4.369512	2.522739	2.000066
H	-2.892728	5.473770	11.322423
H	-3.544263	7.091758	2.000066
H	1.731587	7.091758	2.000066
H	2.412704	4.916404	10.465439
C	-0.189319	3.432397	10.746198
O	10.393270	-0.992649	8.313023
O	10.469023	-0.072697	10.758425
O	11.532239	1.357519	8.731531

O 4.708344 -0.777519 7.922078

O 5.263776 -0.303692 10.545048

O 8.565153 6.090904 8.399217

O 7.959195 4.804316 10.687956

H 4.828273 9.652990 11.437623

H 5.688361 -1.185373 10.467817

H 7.658971 5.473770 11.322423

74

Ru@SiO2-OCHO

Si -0.163631 0.439604 9.239785

Si 2.637872 1.523037 5.062270

Si 2.498901 1.834838 8.210420

Si 0.000053 3.045983 3.985274

Si 5.010657 0.307121 9.149799

Si 7.913722 1.523037 5.062270

Si 7.693655 1.871092 8.246655

Si 5.275903 3.045983 3.985274

Si 7.554967 4.966870 9.174387

Si -0.000053 6.092057 5.062270

Si -0.462766 6.596266 8.126931

Si -2.637872 7.615002 3.985274

Si 5.275797 6.092057 5.062270

Si 5.002287 6.537951 8.225417

Si 2.637979 7.615002 3.985274

O 0.097326 0.146232 10.816525

O 2.709370 1.409217 6.668961

O	0.000053	3.045983	2.370024
O	2.637925	0.000000	4.523772
O	-2.637925	9.138040	4.523772
O	2.824819	3.459347	8.238628
O	3.614086	1.145524	9.168196
O	1.318963	2.284510	4.523772
O	-1.318962	2.284510	4.523772
O	9.232738	2.284510	4.523772
O	0.976732	1.453888	8.623677
O	-0.064257	8.864285	10.664342
O	7.913006	1.551407	6.675124
O	5.275903	3.045983	2.370024
O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	7.668084	3.492527	8.485500
O	8.933918	1.169771	9.034086
O	6.594811	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.258399	1.255219	8.706339
O	-2.615546	4.780889	10.758379
O	0.049854	6.022558	6.693349
O	-2.637872	7.615002	2.370024
O	0.000000	4.569019	4.523772
O	-0.460320	8.222538	8.064451
O	0.608057	6.163348	9.314614
O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772

O	6.594812	6.853530	4.523772
O	-1.937152	5.981844	8.439428
O	5.260820	6.130645	6.679549
O	2.637979	7.615002	2.370024
O	5.275849	4.569019	4.523772
O	5.203097	8.141208	8.450180
O	6.066117	5.641838	9.089345
O	3.956887	6.853530	4.523772
O	1.318963	6.853530	4.523772
O	3.450385	6.195636	8.659127
O	1.368771	3.686630	10.513960
O	-0.076286	2.765466	11.948012
Ru	2.104735	4.933052	9.192619
H	0.125400	0.950080	11.384785
H	-0.906338	2.522739	2.000066
H	0.536331	8.105361	10.749413
H	4.369512	2.522739	2.000066
H	-3.027526	5.401226	11.379213
H	-3.544263	7.091758	2.000066
H	1.731587	7.091758	2.000066
H	-0.250454	4.703522	11.305799
C	0.285047	3.736516	11.301958
O	-0.072752	-0.996832	8.450180
O	-1.617782	1.169771	9.034086
O	4.815530	-0.915502	8.064451
O	5.211593	-0.273754	10.664342
O	8.614548	5.981844	8.439428

O 7.936153 4.780889 10.758379

H 5.812181 -1.032679 10.749413

H 7.524174 5.401226 11.379213

76

Ru@SiO2-OCHO-TS

Si 10.284225 0.355782 9.251226

Si 2.637872 1.523037 5.062270

Si 2.413660 1.779647 8.227621

Si 0.000053 3.045983 3.985274

Si 4.971225 0.333871 9.112335

Si 7.913722 1.523037 5.062270

Si 7.664051 1.875564 8.234764

Si 5.275903 3.045983 3.985274

Si 7.580549 4.949054 9.186029

Si -0.000053 6.092057 5.062270

Si -0.496109 6.655659 8.092838

Si -2.637872 7.615002 3.985274

Si 5.275797 6.092057 5.062270

Si 4.966433 6.445291 8.243805

Si 2.637979 7.615002 3.985274

O -0.026406 0.070356 10.840887

O 2.684749 1.451521 6.674729

O 0.000053 3.045983 2.370024

O 2.637925 0.000000 4.523772

O -2.637925 9.138040 4.523772

O 2.624288 3.408479 8.413042

O	3.570625	1.163353	9.184642
O	1.318963	2.284510	4.523772
O	-1.318962	2.284510	4.523772
O	9.232738	2.284510	4.523772
O	0.933429	1.279871	8.627039
O	-0.057147	8.855177	10.604522
O	7.920828	1.540394	6.673370
O	5.275903	3.045983	2.370024
O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	7.669931	3.492481	8.460408
O	8.856228	1.127208	9.054944
O	6.594811	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.197827	1.298501	8.653997
O	-2.584303	4.727709	10.760457
O	0.030814	6.041493	6.688880
O	-2.637872	7.615002	2.370024
O	0.000000	4.569019	4.523772
O	-0.549984	8.279493	7.998155
O	0.659409	6.371719	9.259488
O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772
O	6.594812	6.853530	4.523772
O	-1.926574	5.992999	8.464429
O	5.256808	6.108293	6.681980
O	2.637979	7.615002	2.370024

O	5.275849	4.569019	4.523772
O	5.064582	8.055965	8.483384
O	6.089475	5.618924	9.097079
O	3.956887	6.853530	4.523772
O	1.318963	6.853530	4.523772
O	3.459928	6.000433	8.687035
O	0.226945	3.792772	9.690249
O	0.323366	3.173590	11.917592
Ru	1.930234	4.967417	9.169420
H	-0.087658	0.838659	11.436327
H	-0.906338	2.522739	2.000066
H	0.488065	8.049258	10.632648
H	4.369512	2.522739	2.000066
H	-2.937281	5.369148	11.395822
H	-3.544263	7.091758	2.000066
H	1.731587	7.091758	2.000066
H	1.512317	4.622127	11.040078
C	0.595623	3.793514	10.910805
O	10.340432	-1.082074	8.483384
O	11.485128	1.279871	8.627039
O	10.525293	0.070356	10.840887
O	4.725866	-0.858546	7.998155
O	5.218703	-0.282863	10.604522
O	8.625126	5.992999	8.464429
O	7.967397	4.727709	10.760457
H	10.464042	0.838659	11.436327
H	5.763915	-1.088781	10.632648

H 7.614418 5.369148 11.395822

177

Ru@SiO2-H-OH-water

Si	5.7036355953	9.4792967452	8.8870257910
Si	2.6380000000	1.5230000000	4.9910000000
Si	3.0153226682	1.7408000636	8.1684330404
Si	0.0000000000	3.0460000000	3.9290000000
Si	0.5066297660	9.4761391346	9.0823450961
Si	7.9140000000	1.5230000000	4.9910000000
Si	8.3345399039	1.9468008784	8.1278208214
Si	5.2760000000	3.0460000000	3.9290000000
Si	-2.2649014523	5.0726170175	9.0194999825
Si	0.0000000000	6.0920000000	4.9910000000
Si	0.3857576624	6.4146795785	8.1329133568
Si	-2.6380000000	7.6150000000	3.9290000000
Si	5.2760000000	6.0920000000	4.9910000000
Si	5.8131285019	6.7022073303	7.9797181833
Si	2.6380000000	7.6150000000	3.9290000000
O	-5.2775986333	8.8792544045	10.3589181991
O	2.6270701399	1.4775629815	6.6084409832
O	0.0000000000	3.0460000000	2.3370000000
O	2.6380000000	0.0000000000	4.4600000000
O	2.7585477173	3.2884781593	8.5353450609
O	-0.7237081865	10.3181121042	8.4158696391
O	1.3190000000	2.2850000000	4.4600000000
O	-1.3190000000	2.2850000000	4.4600000000

O	1.9341022640	0.9347185259	9.1108404026
O	0.0878783648	9.2453729020	10.6569608125
O	7.9135235374	1.5428791769	6.6110789460
O	5.2760000000	3.0460000000	2.3370000000
O	7.9140000000	0.0000000000	4.4600000000
O	8.3173472235	3.5765862737	8.3272636549
O	9.8759249290	1.4800049595	8.4434322761
O	6.5950000000	2.2850000000	4.4600000000
O	3.9570000000	2.2850000000	4.4600000000
O	7.2062549895	1.1720623269	9.0538261805
O	-2.9155802911	4.9595749737	10.5287613493
O	-0.0926118827	6.1051291125	6.6133199988
O	-2.6380000000	7.6150000000	2.3370000000
O	0.0000000000	4.5690000000	4.4600000000
O	0.6858516225	7.9982522891	8.3699849270
O	1.8103922296	5.5911276979	8.3583823389
O	-1.3190000000	6.8540000000	4.4600000000
O	-3.9570000000	6.8540000000	4.4600000000
O	-0.7587244223	5.7470926398	9.1116161693
O	5.2163310503	6.0021559477	6.6229786131
O	2.6380000000	7.6150000000	2.3370000000
O	5.2760000000	4.5690000000	4.4600000000
O	5.8450280529	8.3275656223	7.7223791885
O	7.3394321042	6.0876942574	8.1668614764
O	3.9570000000	6.8540000000	4.4600000000
O	1.3190000000	6.8540000000	4.4600000000
O	4.8647153697	6.4787045936	9.2740139789

O	6.0179946202	4.4984629439	24.1749809704
O	4.6986182359	3.6305559802	21.9263262324
O	6.1833854620	-0.0669005835	19.5841832661
O	8.0207041854	-2.2608969863	15.5710282123
O	6.1151784557	1.2782828955	22.1252692588
O	6.4057892277	2.5670647644	18.5112566115
O	5.2782037310	3.7427235183	10.0697429719
O	0.6563488484	3.6516219833	13.0203585292
O	5.2355247088	5.8713201611	15.8640805113
O	8.6952261581	2.3449402144	17.0343129312
O	0.1583825102	4.5120048593	23.9774470085
O	1.5644082854	5.1616003010	19.4541176483
O	-1.6994946144	8.3558342388	13.7645716406
O	1.9204578210	3.7794855324	21.8421099214
O	-2.8290513591	5.9231547090	14.6595840036
O	4.5094299284	-2.6347543868	19.2169218190
O	2.8752927882	-3.1462550466	21.4778557025
O	0.3023590112	6.8460105949	1.2612446114
O	-0.8692079194	9.0516884631	23.8192139996
O	1.0767648069	4.6995826923	15.4819326982
O	1.7458025823	1.0600110295	12.3321172445
O	3.2918255346	1.8554678258	1.2851472777
O	4.5474410802	3.2839804303	16.6551006724
O	1.9532207874	3.2151755445	17.5969106375
O	-2.1016802927	3.8453744589	12.8773700803
O	-3.3716012359	8.1762859715	22.8504219814
O	7.5413274271	1.6107857835	14.3753293447

O	4.7709137524	1.6437875864	14.5061069758
O	8.7801269878	2.5012256484	22.2705316020
O	1.0207830030	8.1225282429	12.9215595666
O	-1.3302959751	5.0713445080	16.8010807921
O	4.2237820341	2.1259295545	11.9080357909
O	8.3368595095	1.7933858573	1.4510924318
O	0.5383387309	1.3786247523	21.3101301829
O	-4.4546729214	4.9903082228	19.9563259694
O	2.8035587009	7.4062875990	18.4035312049
O	0.3460804816	1.0498905101	18.5039405103
O	5.5001001739	7.2138598415	18.2769322297
O	5.7887904748	6.8703171330	1.0810711523
Ru	3.7166268275	4.8251557762	9.3046040932
H	4.9886257709	7.9264039499	10.2572896320
H	-0.9060000000	2.5230000000	1.9720000000
H	0.6210499960	8.7025121905	11.3029443850
H	4.3700000000	2.5230000000	1.9720000000
H	-2.4989609003	4.4637411603	11.2894024906
H	-3.5440000000	7.0920000000	1.9720000000
H	1.7320000000	7.0920000000	1.9720000000
H	5.4621235671	4.2159276447	23.3995875372
H	5.7320764617	3.9436858370	24.9456462833
H	5.0471749876	4.1890078028	21.1803532165
H	3.7022836508	3.6700646453	21.8968456404
H	6.9741626881	-0.5564337001	19.2302649944
H	5.4539921736	-0.7114108769	19.4556608330
H	7.8150203368	-1.7029931941	14.7977474465

H	8.9754168654	-2.5512372018	15.4843312782
H	5.5660837791	2.0946637348	21.9552091699
H	6.1518244350	0.7875992944	21.2678163461
H	6.2061194643	1.6752799382	18.8911848363
H	5.6903693299	2.7477483668	17.8350094144
H	4.9108759180	3.2250436428	10.8485296002
H	6.0648185803	4.2843891790	10.3683828639
H	3.0313114959	5.0918483901	10.6740638389
H	0.8865486546	4.0484009685	13.9148907888
H	6.0735511681	5.8647710612	15.3192706806
H	5.0379459564	4.9258157951	16.1072361397
H	7.8899662473	2.3531802041	17.6255156855
H	9.3901586304	1.8540759565	17.5357330347
H	0.3242217070	3.9348105495	24.7614992165
H	0.8476377197	4.2913970355	23.2988395760
H	0.6535798521	5.5832202740	19.4174513380
H	2.1495528915	5.9090530357	19.1519404234
H	-2.1294289190	7.5192357081	14.0899991985
H	-2.3835129345	8.8225679711	13.2313237750
H	1.5133687874	2.8991247790	21.6270520598
H	1.7732814531	4.3339639739	21.0285533944
H	-2.3069298031	5.6321896357	15.4629294581
H	-2.6218363611	5.2271654126	13.9798163558
H	3.8912059835	-2.8094046016	19.9685294656
H	4.1329028250	-3.0724112834	18.4113661431
H	2.5140640160	-2.3763272729	22.0109385715
H	3.2355761377	-3.7838795692	22.1219979932

H	0.2583556862	5.9850079458	0.7275624304
H	-0.4794990126	6.8308346427	1.8530364754
H	-0.2088881542	9.4932200627	23.2098205777
H	-0.3902209715	8.3184118355	24.2780018502
H	1.6973672943	5.4804616909	15.4910947624
H	1.4247887380	4.0726142003	16.1778904628
H	1.1760301794	0.6164545459	11.6597872375
H	1.2333076766	1.8357857656	12.6583835082
H	3.6841608285	1.0582288540	0.8143061181
H	2.5794439200	1.5221615063	1.8582463237
H	4.5447250510	2.6824290792	15.8570416009
H	3.6300908550	3.2207760542	17.0392440679
H	1.7759527852	3.8853118515	18.3229270358
H	1.4809968107	2.3844373307	17.8633103601
H	-1.1111498574	3.7568750243	12.9229856352
H	-2.4550128983	3.0158101199	13.2994491211
H	-2.5183632515	8.5204699093	23.2246607837
H	-3.8921850549	7.8624356195	23.6276580751
H	7.9744830457	1.7381336667	15.2524504226
H	6.5670653939	1.6701586167	14.5501687004
H	4.5642455783	1.9523322005	13.5716131830
H	4.3344325583	0.7567470270	14.5416077530
H	8.9523865347	2.8475718173	23.1651446639
H	7.9011638045	2.0531924414	22.3304396125
H	0.0756530088	8.1295417409	13.2252678177
H	1.4182429021	8.9295898290	13.3060856331
H	-1.5279245704	4.1015024245	16.9367533588

H	-0.4479333977	5.0512769832	16.3398315846
H	4.6605952962	1.3308239146	11.4740470503
H	3.2558114068	1.8846202164	11.8675001116
H	8.2583418287	0.8448354837	1.6843476621
H	7.4925246711	2.1968169928	1.7407385654
H	-0.3403892772	1.6461962771	21.7069899094
H	0.8739350942	0.6115103525	21.8261138695
H	-3.6738961604	5.2536074517	20.5151264678
H	-4.2021354179	4.1601674652	19.4772402945
H	3.8062781423	7.3969136643	18.4625054969
H	2.6366098514	7.3634161023	17.4322230668
H	0.4460257747	0.0827283751	18.3471140786
H	0.3700425195	1.1368256854	19.4936409088
H	5.7738213216	6.4911524427	18.8999188914
H	5.5211887903	6.7714844024	17.3847937108
H	5.7862379698	5.9132672407	0.6915374516
H	4.9149057257	7.0253685245	1.4907507461
H	1.0783703014	4.2274394821	12.3576376515
H	1.6949965691	4.6151878179	8.1665694075

73

Pt@SiO2-H-OH

Si	-0.174291	0.385927	9.193502
Si	2.637872	1.523037	5.062270
Si	2.528964	1.767466	8.275928
Si	0.000053	3.045983	3.985274
Si	5.095476	0.309943	9.049096

Si	7.913722	1.523037	5.062270
Si	7.735525	1.935583	8.234064
Si	5.275903	3.045983	3.985274
Si	7.607517	5.042903	9.164884
Si	-0.000053	6.092057	5.062270
Si	-0.448069	6.663889	8.049371
Si	-2.637872	7.615002	3.985274
Si	5.275797	6.092057	5.062270
Si	4.960532	6.523896	8.225551
Si	2.637978	7.615002	3.985274
O	0.039400	0.067883	10.791286
O	2.681408	1.473643	6.689567
O	0.000053	3.045983	2.370024
O	2.637925	0.000000	4.523772
O	-2.637925	9.138040	4.523772
O	3.070800	3.287734	8.612231
O	3.599363	0.903379	9.177353
O	1.318962	2.284510	4.523772
O	-1.318962	2.284510	4.523772
O	9.232738	2.284510	4.523772
O	1.023535	1.408944	8.755861
O	0.242810	8.702649	10.478349
O	7.914801	1.568053	6.675138
O	5.275903	3.045983	2.370024
O	7.913774	0.000000	4.523772
O	2.637925	9.138040	4.523772
O	7.713138	3.554152	8.472777

O	8.950861	1.194305	9.025177
O	6.594812	2.284510	4.523772
O	3.956887	2.284510	4.523772
O	6.275744	1.358106	8.721573
O	-2.448698	4.962075	10.728045
O	0.035951	5.993060	6.680152
O	-2.637872	7.615002	2.370024
O	0.000000	4.569020	4.523772
O	-0.301433	8.276200	7.904799
O	0.664650	6.309315	9.279656
O	-1.318962	6.853530	4.523772
O	-3.956887	6.853530	4.523772
O	6.594812	6.853530	4.523772
O	-1.893777	6.097018	8.462132
O	5.238675	6.084038	6.675307
O	2.637978	7.615002	2.370024
O	5.275849	4.569020	4.523772
O	5.218286	8.164864	8.302550
O	6.136048	5.707889	9.065171
O	3.956887	6.853530	4.523772
O	1.318963	6.853530	4.523772
O	3.509951	6.234759	8.833583
Pt	1.970597	4.802866	8.883070
H	0.722986	3.862241	8.859281
H	4.901408	8.393409	11.122063
H	-0.906338	2.522739	2.000066
H	-0.474186	8.566547	11.119855

H	4.369512	2.522739	2.000066
H	7.759851	4.243676	11.279280
H	-3.544263	7.091758	2.000066
H	1.731587	7.091758	2.000066
H	0.909999	7.079450	9.855160
O	-0.057564	-0.973176	8.302550
O	-1.600839	1.194305	9.025177
O	4.974417	-0.861839	7.904799
O	5.518660	-0.435390	10.478349
O	8.103002	4.962075	10.728045
O	8.657923	6.097018	8.462132
H	-0.374442	-0.744631	11.122063
H	-2.791849	4.243676	11.279280
H	4.801664	-0.571492	11.119855