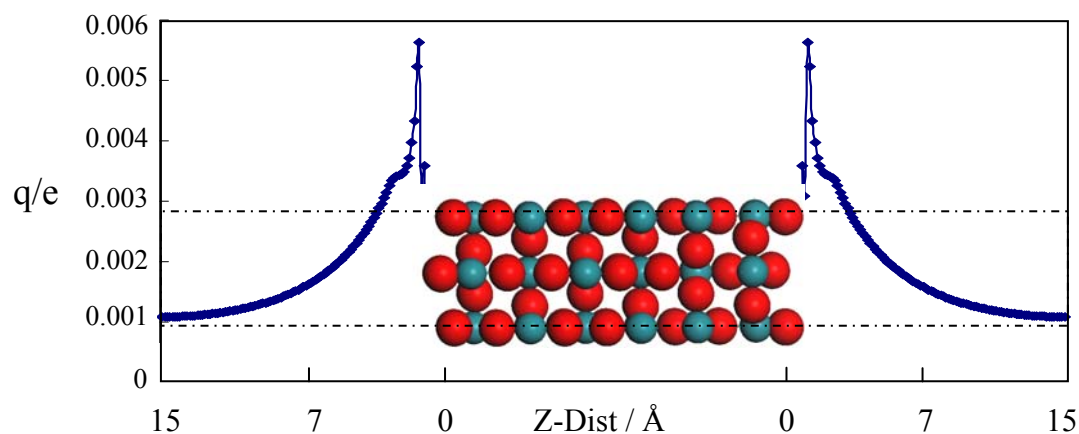


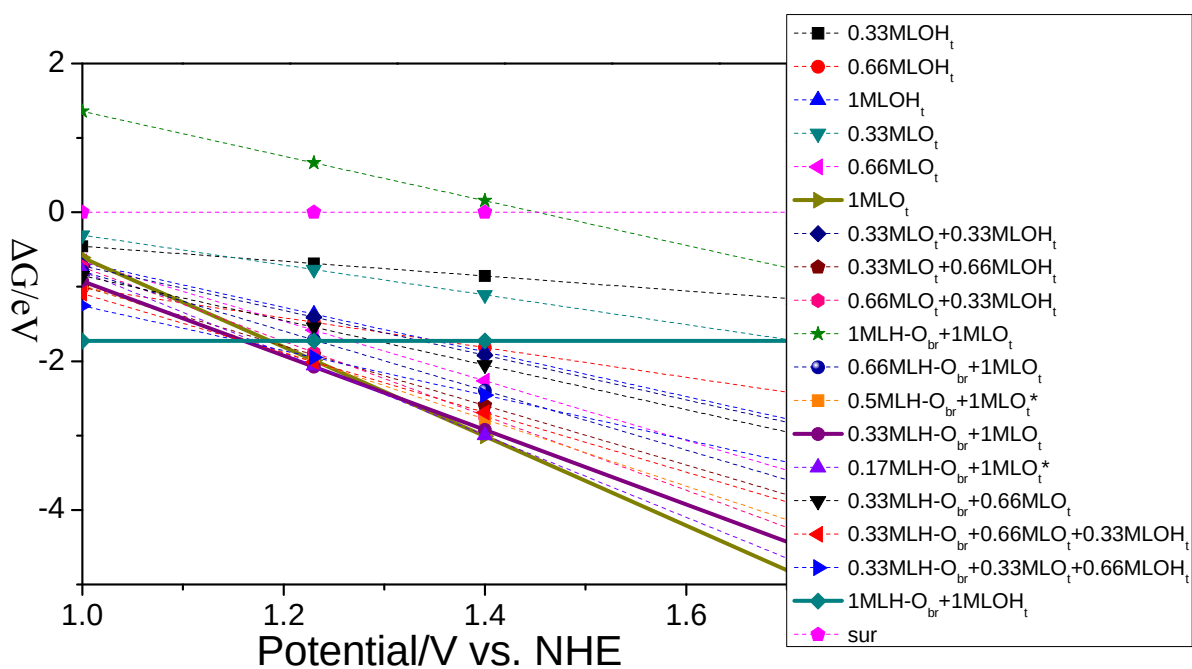
Mechanism and Tafel Lines of Electro-oxidation of Water to Oxygen on $\text{RuO}_2(110)$

Ya-Hui Fang and Zhi-Pan Liu*

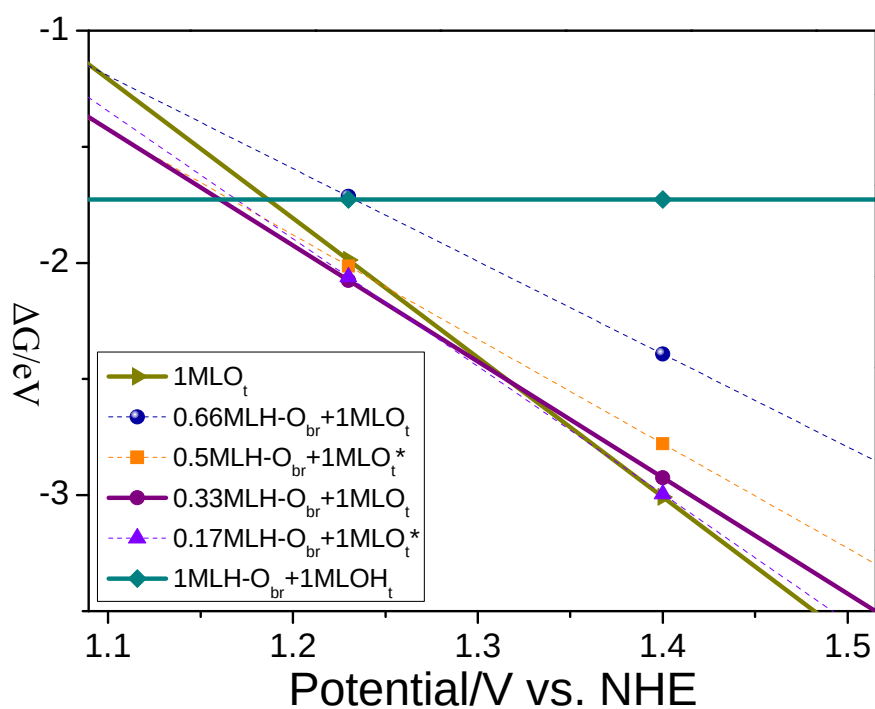
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S-Figure 1 An example showing the ionic countercharge distribution (total $q=0.4e$) on O-terminated $\text{RuO}_2(110)$ at the Z-direction as solved from modified Poisson-Boltzmann equation



S-Figure 2 The surface phase diagram of $\text{RuO}_2(110)$ surface calculated in vacuum.



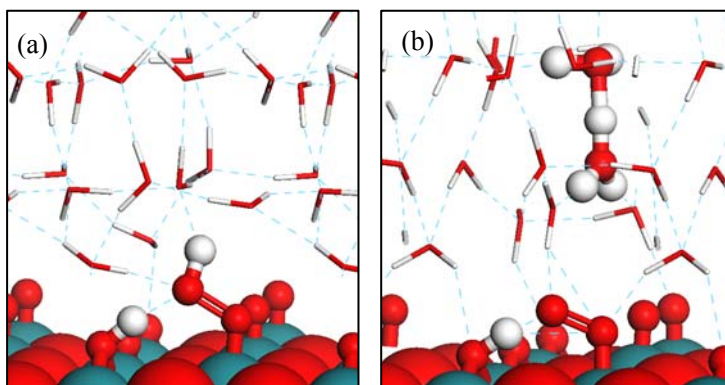
S-Figure 3 An enlarged local view of S-Figure 2 to show more clearly the OH/O phases.

S-Table 1 Convergence of k-point mesh for the calculated free energies of elementary steps in OER on the O-terminated phase of RuO₂(110).

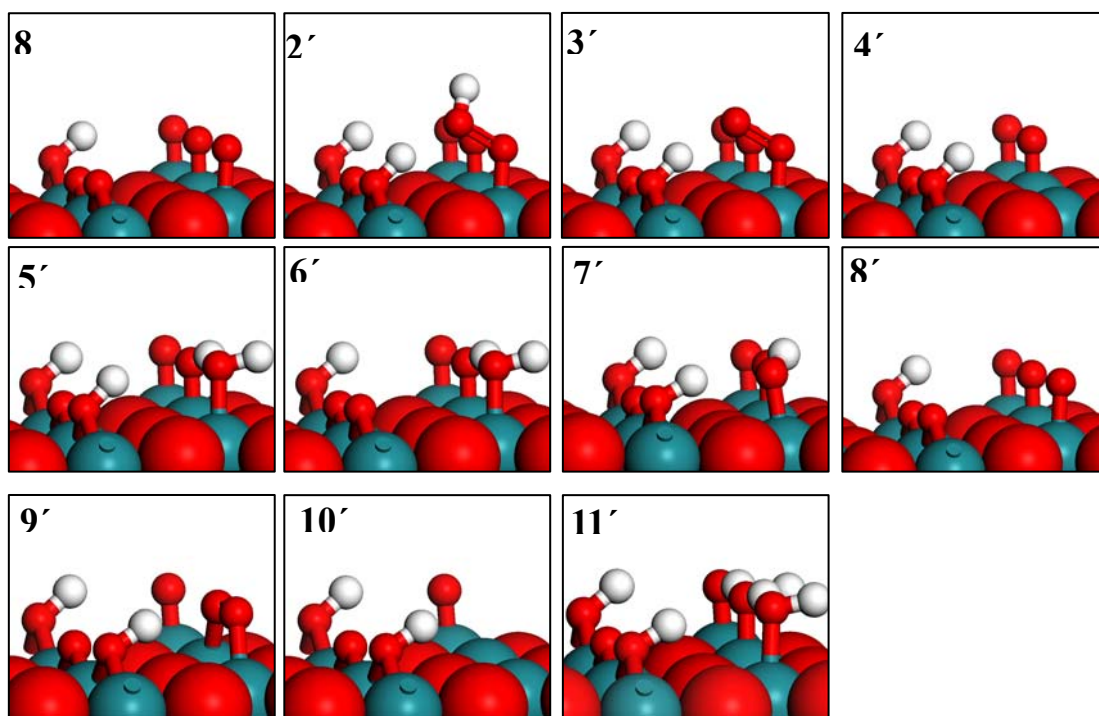
elementary steps	ΔE	$\Delta H(0 \rightarrow 298K)$	ΔZPE	$-T\Delta S$	$- e U$	ΔG
(2×3×1) k-point mesh						
1→2	0.03	0	0.03	0.22	0	0.28
2 →3+ H⁺ + e⁻	1.68	0.04	-0.15	-0.2	-1.58	-0.20
3→4+O₂	0.25	0.09	-0.08	-0.64	0	-0.38
4+H₂O→ 5	-0.59	0	0.17	0.22	0	-0.20
5→6 + H⁺ + e⁻	1.53	0.04	-0.21	-0.2	-1.58	-0.42
6→7	0.16	0	-0.03	0	0	0.13
(3×4×1) k-point mesh						
1→2	0.09	0	0.03	0.22	0	0.34
2 →3+ H⁺ + e⁻	1.74	0.04	-0.15	-0.2	-1.58	-0.15
3→4+O₂	0.23	0.09	-0.08	-0.64	0	-0.40
4+H₂O→ 5	-0.62	0	0.17	0.22	0	-0.23
5→6 + H⁺ + e⁻	1.58	0.04	-0.21	-0.2	-1.58	-0.36
6→7	0.09	0	-0.03	0	0	0.06

S-Table.2 Reaction barriers (E_a) for oxygen coupling reactions on RuO₂(110).

Reaction path	Surface coverage	E_{a1} (eV) (O(H) _{br} ⁺ O(H) _t)	E_{a2} (eV) (O(H) _t +O(H) _t)
O+O reaction	1MLO _{br} + 0.33MLO _t	0.94	-----
	1MLO _{br} +0.67MLO _t	1.13	0.84
	1MLO _{br} +1MLO _t	0.90	0.64
	1MLO _{br} +0.33MLO _t + 0.33MLOH _t	0.93	-----
	1MLO _{br} +0.33MLO _t + 0.67MLOH _t	1.08	-----
	1MLO _{br} +0.67MLO _t + 0.33MLOH _t	1.11	0.72
O+OH reaction	1ML O _{br} +0.67MLOH _t	1.42	-----
	1ML O _{br} +1MLOH _t	1.45	-----
	1ML O _{br} +0.33MLO _t + 0.33MLOH _t	1.17	0.83
	1ML O _{br} +0.33MLO _t + 0.67MLOH _t	1.22	1.10
	1ML O _{br} +0.67MLO _t + 0.33MLOH _t	1.23	1.10
OH+OH reaction	O _{br} +1MLOH _t	-----	1.5



S-Figure 4 The snapshots for the deprotonation of OOH from first-principles molecular dynamics simulation. **(a)**: the initial state (OOH on the surface). **(b)**: the deprotonated O_2 plus a $H_5O_2^+$ in solution. The MD simulation is performed with a Nose thermostat at 330 K ($\Delta t = 1$ fs) by including three-layer water on the surface. The MD simulation shows that the proton transfer from the HOO-Ru_{5c} to the water layers occurs within ~ 0.5 ps leading to a $H_5O_2^+$ in solution.



S-Figure 5 the Optimized structures for intermediate states for OER on the OH/O mixed phase of RuO₂(110) at 1.4 V. For the optimized structures, the first H₂O layer is omitted for clarity. O: Red ball; H: white ball; Ru: Green ball.

S-Table 3 The optimized XYZ coordinates (in Å) for the OH-terminated phase and the OH/O mixed phase

XYZ Coordinates							
OH-terminated phase				OH/O mixed phase			
H	13.2195	6.5373	34.6026	H	1.1936	2.1047	11.8335
H	12.3516	8.4269	34.0045	H	4.0447	2.1379	11.9910
H	7.0916	6.5649	34.5835	H	7.2214	2.1521	11.9550
H	6.1680	8.4720	33.9805	H	0.2428	1.3358	10.8287
H	10.1928	6.5543	34.5812	H	3.2813	1.3885	10.8178
H	9.2825	8.4672	33.9773	H	6.3943	1.4024	10.8300
H	9.2491	11.6615	14.4116	H	1.0938	0.5218	9.1277
H	8.4133	9.8509	13.7423	H	4.2100	0.5333	9.1526
H	12.3366	11.6193	14.3668	H	7.2758	0.5386	9.1398
H	11.5445	9.8339	13.7257	H	0.2562	-0.6674	9.7061
H	6.1289	11.6544	14.4143	H	3.3550	-0.6527	9.7114
H	5.2611	9.8783	13.7770	H	6.4378	-0.6522	9.7110
H	1.0232	2.0568	11.9675	H	1.3406	3.9418	9.3653
H	4.1119	2.0595	11.9702	H	4.4109	3.9523	9.3338
H	7.1995	2.0558	11.9700	H	7.5063	3.9575	9.3295
H	0.1803	1.3990	10.8058	H	0.3346	3.4028	10.4520
H	3.2695	1.4002	10.8084	H	3.4124	3.4227	10.4374
H	6.3631	1.3958	10.8043	H	6.5146	3.4267	10.4385
H	1.0755	0.5912	9.1026	H	0.7789	3.6403	38.6182
H	4.1689	0.5909	9.1057	H	3.8924	3.6816	38.6303
H	7.2575	0.5908	9.1033	H	6.8786	3.6684	38.6843
H	0.2515	-0.5994	9.6956	H	-0.1099	4.8284	38.1446
H	3.3418	-0.5990	9.6953	H	2.9864	4.8764	38.1867
H	6.4325	-0.6012	9.6930	H	6.0576	4.9181	38.2103
H	1.3415	3.9900	9.3915	H	0.9073	0.3053	38.6634
H	4.4277	3.9870	9.3872	H	3.9655	0.2769	38.7755
H	7.5220	3.9874	9.3940	H	7.0739	0.2997	38.7697
H	0.3453	3.4481	10.4880	H	-0.0180	0.7290	37.4757
H	3.4341	3.4468	10.4868	H	3.0333	0.7670	37.6042
H	6.5239	3.4452	10.4885	H	6.1235	0.7885	37.6079
H	0.7253	3.6348	38.6422	H	1.1331	2.0040	36.0894
H	3.8178	3.6348	38.6378	H	3.5801	1.9194	35.8585
H	6.8982	3.6345	38.6455	H	6.6698	1.9345	35.8194
H	-0.1152	4.8770	38.1955	H	-0.0022	2.8667	36.7814
H	2.9769	4.8794	38.1969	H	2.9399	2.7978	37.0365
H	6.0650	4.8814	38.1972	H	6.0196	2.7983	36.9953
H	0.9154	0.2771	38.7604	H	9.3014	7.1739	14.0835
H	4.0064	0.2734	38.7661	H	9.2478	2.7076	34.5859

H	7.1016	0.2780	38.7593	O	0.0341	0.0282	14.7300
H	-0.0257	0.7865	37.6033	O	3.1203	0.0621	15.0898
H	3.0688	0.7865	37.6089	O	6.2230	0.0613	15.0868
H	6.1595	0.7886	37.6040	O	0.0233	3.2327	18.0642
H	0.7670	1.9730	36.0420	O	3.1069	3.2300	18.0944
H	3.8575	1.9791	36.0491	O	6.2113	3.2327	18.1001
H	6.9619	1.9788	36.0466	O	3.0701	6.3710	27.7925
H	-0.1312	2.8157	37.0312	O	6.1599	6.3738	27.7913
H	2.9581	2.8128	37.0440	O	9.2520	6.3728	27.7746
H	6.0531	2.8186	37.0292	O	3.0438	3.1402	30.9660
O	-0.0338	-0.1842	14.8641	O	6.1638	3.1411	30.9649
O	3.0458	-0.1941	14.7722	O	9.2395	3.1413	30.9248
O	6.1166	-0.1873	14.8649	O	0.0347	0.0550	17.4918
O	-0.0507	3.0958	18.0924	O	3.1121	0.0507	17.4579
O	3.0362	3.0953	18.0970	O	6.2235	0.0502	17.4601
O	6.1250	3.0941	18.0950	O	0.0182	3.2146	20.6391
O	0.0350	-0.0204	27.7742	O	3.1096	3.2154	20.6240
O	3.1283	-0.0221	27.7727	O	6.1994	3.2186	20.6220
O	6.2208	-0.0195	27.7741	O	3.0604	-0.0293	30.3225
O	0.0503	3.2308	30.9892	O	6.1663	-0.0263	30.3221
O	3.1351	3.2161	30.9457	O	9.2466	-0.0325	30.3526
O	6.2110	3.2341	30.9950	O	3.0524	3.1299	33.3443
O	-0.0386	0.0531	17.3984	O	6.1543	3.1310	33.3407
O	3.0385	0.0353	17.4552	O	9.2323	3.1688	33.6526
O	6.1219	0.0497	17.4037	O	1.5574	4.4876	16.1606
O	-0.0449	3.1789	20.6274	O	4.6750	4.4767	16.2270
O	3.0470	3.1769	20.6291	O	7.7878	4.4903	16.1683
O	6.1407	3.1781	20.6276	O	1.5669	1.2680	19.4231
O	0.0515	-0.1035	30.2922	O	4.6569	1.2545	19.4078
O	3.1401	-0.1018	30.2889	O	7.7466	1.2673	19.4235
O	6.2271	-0.1021	30.2939	O	1.5232	4.4263	29.0075
O	0.0492	2.9974	33.5313	O	4.6109	4.4125	29.0205
O	3.1229	2.9865	33.6098	O	7.7024	4.4297	29.0068
O	6.2025	3.0000	33.5303	O	1.4878	1.1677	32.2506
O	1.4946	4.4253	16.2584	O	4.5978	1.1581	32.2027
O	4.5774	4.4317	16.2815	O	7.7085	1.1687	32.2487
O	7.6705	4.4174	16.2619	O	1.5762	2.0282	16.1847
O	1.4978	1.2102	19.4180	O	4.6761	2.0379	16.2151
O	4.5902	1.2099	19.4185	O	7.7683	2.0261	16.1918
O	7.6784	1.2063	19.4034	O	1.5660	5.1587	19.4080
O	1.5858	4.4018	28.9869	O	4.6584	5.1765	19.4022
O	4.6767	4.4028	28.9867	O	7.7488	5.1640	19.4087
O	7.7665	4.3993	28.9987	O	1.5235	1.9281	28.9926
O	1.5989	1.2143	32.1122	O	4.6133	1.9437	29.0074

O	4.6853	1.2080	32.1318	O	7.7033	1.9290	28.9919
O	7.7783	1.2035	32.1251	O	1.4943	5.0983	32.2315
O	1.4931	1.9438	15.9780	O	4.5987	5.1081	32.1981
O	4.5793	1.9336	15.9875	O	7.7017	5.1007	32.2275
O	7.6712	1.9465	15.9824	O	1.5450	4.4120	22.6081
O	1.4960	5.1151	19.3799	O	4.6350	4.4120	22.6081
O	4.5911	5.1143	19.3819	O	7.7250	4.4120	22.6081
O	7.6795	5.1210	19.3563	O	1.5450	1.2159	25.8042
O	1.5841	1.9144	29.0177	O	4.6350	1.2159	25.8042
O	4.6793	1.9150	29.0196	O	7.7250	1.2159	25.8042
O	7.7660	1.9219	29.0431	O	1.5450	1.9803	22.6081
O	1.5985	5.1070	32.3805	O	4.6350	1.9803	22.6081
O	4.6852	5.1176	32.3904	O	7.7250	1.9803	22.6081
O	7.7763	5.1189	32.3824	O	1.5450	5.1764	25.8042
O	1.5450	4.4120	22.6081	O	4.6350	5.1764	25.8042
O	4.6350	4.4120	22.6081	O	7.7250	5.1764	25.8042
O	7.7250	4.4120	22.6081	O	0.0000	0.0000	21.3922
O	1.5450	1.2159	25.8042	O	3.0900	0.0000	21.3922
O	4.6350	1.2159	25.8042	O	6.1800	0.0000	21.3922
O	7.7250	1.2159	25.8042	O	0.0000	3.1961	24.5884
O	1.5450	1.9803	22.6081	O	3.0900	3.1961	24.5884
O	4.6350	1.9803	22.6081	O	6.1800	3.1961	24.5884
O	7.7250	1.9803	22.6081	O	0.0000	0.0000	23.8240
O	1.5450	5.1764	25.8042	O	3.0900	0.0000	23.8240
O	4.6350	5.1764	25.8042	O	6.1800	0.0000	23.8240
O	7.7250	5.1764	25.8042	O	0.0000	3.1961	27.0201
O	0.0000	0.0000	21.3922	O	3.0900	3.1961	27.0201
O	3.0900	0.0000	21.3922	O	6.1800	3.1961	27.0201
O	6.1800	0.0000	21.3922	O	3.0807	6.3338	34.1566
O	0.0000	3.1961	24.5884	O	6.1340	6.3351	34.1572
O	3.0900	3.1961	24.5884	O	9.2353	6.3030	34.2064
O	6.1800	3.1961	24.5884	O	0.0203	3.1444	14.2208
O	0.0000	0.0000	23.8240	O	3.1614	3.2615	14.2607
O	3.0900	0.0000	23.8240	O	6.2050	3.2663	14.2621
O	6.1800	0.0000	23.8240	O	0.2536	2.0815	11.5198
O	0.0000	3.1961	27.0201	O	3.2042	2.1617	11.4767
O	3.0900	3.1961	27.0201	O	6.3602	2.1835	11.4781
O	6.1800	3.1961	27.0201	O	0.2100	0.3297	9.5222
O	12.3382	6.7581	34.2079	O	3.3190	0.3472	9.5360
O	6.1943	6.7632	34.2104	O	6.3932	0.3489	9.5392
O	9.2967	6.7600	34.2077	O	0.4154	4.0654	9.6872
O	9.2827	10.0687	14.1605	O	3.4899	4.0812	9.6639
O	12.3996	10.0689	14.1610	O	6.5875	4.0880	9.6631
O	6.1519	10.0737	14.1668	O	-0.1065	3.8230	38.2222

O	0.1610	2.1456	11.4972	O	2.9912	3.8639	38.2688
O	3.2499	2.1486	11.4976	O	6.0154	3.9023	38.2702
O	6.3406	2.1430	11.4950	O	-0.0079	0.1817	38.3083
O	0.1920	0.3931	9.4950	O	3.0606	0.1405	38.4031
O	3.2837	0.3936	9.4958	O	6.1620	0.1682	38.4178
O	6.3730	0.3913	9.4934	O	0.1319	2.1360	36.0920
O	0.4274	4.1298	9.7347	O	2.8141	1.9525	36.4771
O	3.5144	4.1288	9.7339	O	5.9398	1.9351	36.4743
O	6.6077	4.1278	9.7356	Ru	0.0000	3.1961	22.6081
O	-0.1576	3.8648	38.2675	Ru	3.0900	3.1961	22.6081
O	2.9331	3.8663	38.2683	Ru	6.1800	3.1961	22.6081
O	6.0182	3.8688	38.2675	Ru	0.0000	0.0000	25.8042
O	0.0117	0.1386	38.3899	Ru	3.0900	0.0000	25.8042
O	3.1047	0.1322	38.3923	Ru	6.1800	0.0000	25.8042
O	6.1972	0.1405	38.3902	Ru	1.5450	0.0000	22.6081
O	-0.1197	1.9659	36.4728	Ru	4.6350	0.0000	22.6081
O	2.9779	1.9582	36.4913	Ru	7.7250	0.0000	22.6081
O	6.0724	1.9687	36.4727	Ru	1.5450	3.1961	25.8042
Ru	0.0000	3.1961	22.6081	Ru	4.6350	3.1961	25.8042
Ru	3.0900	3.1961	22.6081	Ru	7.7250	3.1961	25.8042
Ru	6.1800	3.1961	22.6081	Ru	0.0422	3.2633	15.9427
Ru	0.0000	0.0000	25.8042	Ru	3.1277	3.2573	15.9779
Ru	3.0900	0.0000	25.8042	Ru	6.2288	3.2579	15.9782
Ru	6.1800	0.0000	25.8042	Ru	3.0559	3.1768	28.9968
Ru	1.5450	0.0000	22.6081	Ru	6.1696	3.1794	28.9983
Ru	4.6350	0.0000	22.6081	Ru	9.2465	3.1784	28.9767
Ru	7.7250	0.0000	22.6081	Ru	1.5543	3.2109	19.3458
Ru	1.5450	3.1961	25.8042	Ru	4.6565	3.2161	19.3522
Ru	4.6350	3.1961	25.8042	Ru	7.7608	3.2142	19.3455
Ru	7.7250	3.1961	25.8042	Ru	1.4753	3.1301	32.2539
Ru	-0.0454	3.1884	16.1200	Ru	4.6004	3.1304	32.2289
Ru	3.0445	3.1885	16.1326	Ru	7.7344	3.1312	32.2523
Ru	6.1193	3.1879	16.1245	Ru	0.0245	0.0181	19.4393
Ru	0.0432	3.1638	29.0124	Ru	3.1007	0.0169	19.4192
Ru	3.1303	3.1603	28.9890	Ru	6.2132	0.0191	19.4222
Ru	6.2173	3.1645	29.0168	Ru	3.0418	6.3253	32.4309
Ru	1.4954	3.1614	19.3632	Ru	6.1417	6.3281	32.4326
Ru	4.5867	3.1609	19.3654	Ru	9.2271	6.3256	32.4845
Ru	7.6766	3.1628	19.3592	Ru	1.5427	0.0667	16.1714
Ru	1.6140	3.1621	32.2243	Ru	4.6737	0.0649	16.1929
Ru	4.6404	3.1649	32.2318	Ru	7.7911	0.0665	16.1765
Ru	7.7680	3.1625	32.2154	Ru	1.5074	6.3732	29.0723
Ru	-0.0419	-0.0278	19.3861	Ru	4.6125	6.3755	29.0636
Ru	3.0452	-0.0315	19.4177	Ru	7.7174	6.3762	29.0691

Ru	6.1321	-0.0285	19.3886		
Ru	0.0578	-0.0348	32.2572		
Ru	3.1349	-0.0344	32.2488		
Ru	6.2268	-0.0331	32.2606		
Ru	1.5354	-0.0094	16.1526		
Ru	4.5504	-0.0131	16.1587		
Ru	7.6731	-0.0153	16.1716		
Ru	1.5900	-0.0389	29.0289		
Ru	4.6809	-0.0382	29.0295		
Ru	7.7688	-0.0365	29.0346		

S-Table 4 The optimized XYZ coordinates (in Å) for O-terminated phase and the TS structures of Water dissociation (TS1) and O coupling (TS2) as shown in Figure 2.

XYZ Coordinates									
Atom	O-terminated phase(IS)			Water dissociation (TS1)			O coupling (TS2)		
H	1.0451	2.0653	11.9862	1.0489	2.0883	11.9705	1.0558	2.1012	11.9372
H	4.1300	2.0661	11.9883	4.1299	2.0863	11.9745	4.1431	2.1006	11.9392
H	7.2257	2.0623	11.9880	7.2270	2.0856	11.9700	7.2344	2.0985	11.9384
H	0.2082	1.3953	10.8227	0.2070	1.4044	10.8181	0.1973	1.3955	10.8100
H	3.2966	1.3963	10.8227	3.2917	1.4027	10.8191	3.2870	1.3954	10.8099
H	6.3864	1.3938	10.8261	6.3856	1.4028	10.8168	6.3771	1.3928	10.8101
H	1.0638	0.6202	9.0823	1.0750	0.6047	9.0992	1.0836	0.5709	9.1140
H	4.1589	0.6183	9.0818	4.1660	0.6039	9.0986	4.1767	0.5696	9.1162
H	7.2503	0.6191	9.0805	7.2579	0.6043	9.0968	7.2645	0.5688	9.1151
H	0.2595	-0.5814	9.6838	0.2615	-0.5915	9.6966	0.2485	-0.6118	9.7081
H	3.3503	-0.5811	9.6824	3.3483	-0.5914	9.6920	3.3381	-0.6114	9.7082
H	6.4392	-0.5778	9.6787	6.4387	-0.5907	9.6879	6.4287	-0.6141	9.7081
H	1.3439	3.9822	9.3900	1.3445	3.9907	9.3860	1.3365	3.9916	9.3915
H	4.4290	3.9803	9.3865	4.4307	3.9865	9.3825	4.4235	3.9899	9.3889
H	7.5270	3.9799	9.3931	7.5261	3.9897	9.3863	7.5177	3.9898	9.3926
H	0.3526	3.4646	10.4983	0.3506	3.4626	10.4900	0.3344	3.4471	10.4833
H	3.4367	3.4645	10.4945	3.4349	3.4601	10.4859	3.4236	3.4464	10.4831
H	6.5316	3.4643	10.4982	6.5284	3.4608	10.4862	6.5144	3.4449	10.4831
H	0.7100	3.6018	38.6323	0.7559	3.6293	38.6532	0.7533	3.6517	38.6333
H	3.8045	3.6034	38.6312	3.9548	3.7309	38.6040	3.8424	3.6485	38.6294
H	6.8858	3.6034	38.6358	6.8549	3.6250	38.6486	6.9126	3.6495	38.6412
H	-0.1276	4.8467	38.2093	-0.1085	4.8481	38.1835	-0.1142	4.8697	38.1747
H	2.9671	4.8477	38.2069	2.8865	4.6851	38.0406	2.9748	4.8657	38.1747
H	6.0537	4.8514	38.2122	6.0685	4.8843	38.1536	6.0596	4.8741	38.1748
H	0.9171	0.3155	38.7840	0.8541	0.3130	38.7705	0.9117	0.2686	38.7292
H	4.0095	0.3144	38.7836	7.0360	0.3030	38.7474	3.9992	0.2676	38.7307
H	7.1045	0.3166	38.7825	-0.0409	0.7670	37.5590	7.0906	0.2688	38.7330

H	-0.0008	0.7610	37.5874	6.2230	0.8020	37.4718	-0.0341	0.7653	37.5714
H	3.0898	0.7583	37.5877	0.6629	1.8527	35.8207	3.0544	0.7627	37.5708
H	6.1832	0.7616	37.5887	6.9983	1.9473	35.9328	6.1521	0.7678	37.5690
H	0.7601	1.9064	35.8795	-0.0766	2.7650	36.9152	0.7777	1.9451	35.9870
H	3.8504	1.9068	35.8785	6.0591	2.7674	36.9029	3.7975	1.9187	35.9201
H	6.9476	1.9113	35.8815	3.0150	2.4298	34.3600	6.9625	1.9450	35.9759
H	-0.1085	2.7667	36.8850	3.3482	1.1504	35.9205	-0.1284	2.7846	36.9751
H	2.9820	2.7663	36.8843	4.3019	0.5031	38.3017	2.9608	2.7674	36.9640
H	6.0742	2.7697	36.8838	3.1564	1.5481	38.0899	6.0540	2.7709	36.9677
O	0.0568	0.0414	15.0081	0.0596	0.0386	15.0109	0.0619	0.0400	15.0379
O	3.1454	0.0426	15.0042	3.1477	0.0387	15.0069	3.1507	0.0389	15.0096
O	6.2358	0.0427	15.0142	6.2382	0.0383	15.0164	6.2388	0.0403	15.0305
O	0.0412	3.2225	18.0937	0.0445	3.2203	18.0935	0.0475	3.2202	18.0960
O	3.1316	3.2212	18.0944	3.1340	3.2198	18.0970	3.1375	3.2202	18.0984
O	6.2214	3.2224	18.0921	6.2239	3.2196	18.0919	6.2273	3.2203	18.0975
O	3.0536	6.3758	27.7891	3.0516	6.3746	27.7914	3.0388	6.3768	27.7912
O	6.1439	6.3786	27.7881	6.1452	6.3792	27.7896	6.1629	6.3730	27.7895
O	9.2339	6.3775	27.7877	9.2327	6.3766	27.7891	9.2374	6.3714	27.7265
O	3.0350	3.1733	30.9555	3.0368	3.1672	30.9270	2.9620	3.1504	30.9426
O	6.1249	3.1753	30.9539	6.1349	3.1660	30.9590	6.2179	3.1575	30.9507
O	9.2161	3.1768	30.9549	9.2126	3.1733	30.9631	9.2135	3.1642	30.9932
O	0.0525	0.0172	17.4610	0.0549	0.0200	17.4651	0.0550	0.0364	17.4731
O	3.1451	0.0182	17.4617	3.1477	0.0204	17.4658	3.1470	0.0370	17.4784
O	6.2338	0.0196	17.4598	6.2373	0.0208	17.4634	6.2420	0.0363	17.4746
O	0.0334	3.2092	20.6309	0.0367	3.2087	20.6314	0.0392	3.2160	20.6325
O	3.1243	3.2078	20.6306	3.1267	3.2086	20.6296	3.1292	3.2160	20.6317
O	6.2141	3.2100	20.6311	6.2161	3.2088	20.6320	6.2193	3.2161	20.6320
O	3.0471	0.0027	30.3314	3.0520	6.3714	30.3102	2.9947	-0.0089	30.2303
O	6.1377	0.0026	30.3334	6.1342	6.3991	30.3389	6.2080	-0.0142	30.2340
O	9.2271	0.0020	30.3343	9.2288	6.4008	30.3484	9.2276	-0.0090	30.4515
O	3.0340	3.2250	33.4002	3.0455	3.2544	33.6210	3.0986	3.1809	33.4352
O	6.1236	3.2237	33.4120	6.1175	3.2131	33.3369	6.0734	3.1818	33.4102
O	9.2129	3.2216	33.4078	9.2240	3.2295	33.3455	9.2223	3.1755	33.4047
O	1.6005	4.4390	16.1973	1.6019	4.4397	16.2030	1.6048	4.4457	16.2245
O	4.6899	4.4376	16.1961	4.6907	4.4391	16.2011	4.6915	4.4460	16.2247
O	7.7795	4.4380	16.1957	7.7815	4.4390	16.2006	7.7820	4.4450	16.2230
O	1.5830	1.2593	19.4094	1.5861	1.2599	19.4150	1.5887	1.2682	19.4235
O	4.6734	1.2603	19.4090	4.6767	1.2599	19.4150	4.6798	1.2679	19.4238
O	7.7634	1.2603	19.4082	7.7662	1.2607	19.4147	7.7694	1.2678	19.4235
O	1.5045	4.4278	29.0137	1.5020	4.4262	29.0042	1.4920	4.4245	29.0070
O	4.5940	4.4279	29.0136	4.5964	4.4239	29.0015	4.5947	4.4121	29.0074
O	7.6843	4.4291	29.0118	7.6832	4.4256	29.0133	7.6988	4.4253	29.0004
O	1.4843	1.2210	32.2540	1.4925	1.2380	32.3240	1.5211	1.1943	32.3937
O	4.5771	1.2217	32.2497	4.5567	1.2301	32.2873	4.5837	1.2397	31.9306

O	7.6661	1.2210	32.2577	7.6692	1.2139	32.2942	7.6462	1.1916	32.3980
O	1.5999	1.9909	16.2257	1.6016	1.9919	16.2208	1.6046	1.9992	16.2098
O	4.6896	1.9903	16.2215	4.6907	1.9923	16.2201	4.6913	1.9986	16.2109
O	7.7809	1.9910	16.2218	7.7824	1.9926	16.2190	7.7825	2.0004	16.2089
O	1.5836	5.1641	19.4108	1.5865	5.1650	19.4140	1.5893	5.1720	19.4156
O	4.6738	5.1645	19.4094	4.6770	5.1651	19.4139	4.6800	5.1722	19.4157
O	7.7633	5.1648	19.4085	7.7663	5.1644	19.4142	7.7698	5.1721	19.4157
O	1.5046	1.9398	29.0035	1.5024	1.9348	28.9952	1.4905	1.9358	28.9917
O	4.5951	1.9398	29.0027	4.5954	1.9359	28.9923	4.5972	1.9466	28.9964
O	7.6853	1.9400	29.0035	7.6847	1.9402	29.0054	7.7002	1.9346	28.9886
O	1.4878	5.1684	32.1977	1.5012	5.1703	32.2111	1.5285	5.1471	32.3538
O	4.5767	5.1687	32.1979	4.5797	5.1553	32.2229	4.5805	5.1077	31.8911
O	7.6661	5.1673	32.1963	7.6628	5.1706	32.1984	7.6432	5.1472	32.3596
O	1.5450	4.4120	22.6081	1.5450	4.4120	22.6081	1.5450	4.4120	22.6081
O	4.6350	4.4120	22.6081	4.6350	4.4120	22.6081	4.6350	4.4120	22.6081
O	7.7250	4.4120	22.6081	7.7250	4.4120	22.6081	7.7250	4.4120	22.6081
O	1.5450	1.2159	25.8042	1.5450	1.2159	25.8042	1.5450	1.2159	25.8042
O	4.6350	1.2159	25.8042	4.6350	1.2159	25.8042	4.6350	1.2159	25.8042
O	7.7250	1.2159	25.8042	7.7250	1.2159	25.8042	7.7250	1.2159	25.8042
O	1.5450	1.9803	22.6081	1.5450	1.9803	22.6081	1.5450	1.9803	22.6081
O	4.6350	1.9803	22.6081	4.6350	1.9803	22.6081	4.6350	1.9803	22.6081
O	7.7250	1.9803	22.6081	7.7250	1.9803	22.6081	7.7250	1.9803	22.6081
O	1.5450	5.1764	25.8042	1.5450	5.1764	25.8042	1.5450	5.1764	25.8042
O	4.6350	5.1764	25.8042	4.6350	5.1764	25.8042	4.6350	5.1764	25.8042
O	7.7250	5.1764	25.8042	7.7250	5.1764	25.8042	7.7250	5.1764	25.8042
O	0.0000	0.0000	21.3922	0.0000	0.0000	21.3922	0.0000	0.0000	21.3922
O	3.0900	0.0000	21.3922	3.0900	0.0000	21.3922	3.0900	0.0000	21.3922
O	6.1800	0.0000	21.3922	6.1800	0.0000	21.3922	6.1800	0.0000	21.3922
O	0.0000	3.1961	24.5884	0.0000	3.1961	24.5884	0.0000	3.1961	24.5884
O	3.0900	3.1961	24.5884	3.0900	3.1961	24.5884	3.0900	3.1961	24.5884
O	6.1800	3.1961	24.5884	6.1800	3.1961	24.5884	6.1800	3.1961	24.5884
O	0.0000	0.0000	23.8240	0.0000	0.0000	23.8240	0.0000	0.0000	23.8240
O	3.0900	0.0000	23.8240	3.0900	0.0000	23.8240	3.0900	0.0000	23.8240
O	6.1800	0.0000	23.8240	6.1800	0.0000	23.8240	6.1800	0.0000	23.8240
O	0.0000	3.1961	27.0201	0.0000	3.1961	27.0201	0.0000	3.1961	27.0201
O	3.0900	3.1961	27.0201	3.0900	3.1961	27.0201	3.0900	3.1961	27.0201
O	6.1800	3.1961	27.0201	6.1800	3.1961	27.0201	6.1800	3.1961	27.0201
O	3.0374	6.3240	34.1776	0.0620	3.1972	14.2610	3.7628	6.3311	33.9998
O	6.1246	6.3177	34.1788	3.1492	3.1947	14.2617	5.4112	6.3266	33.9961
O	9.2166	6.3123	34.1796	6.2400	3.1939	14.2598	9.2184	6.3134	34.3102
O	0.0594	3.1847	14.2618	0.1818	2.1549	11.5036	0.0612	3.2518	14.2658
O	3.1478	3.1818	14.2626	3.2648	2.1532	11.5045	3.1511	3.2503	14.2642
O	6.2383	3.1801	14.2594	6.3598	2.1520	11.5034	6.2385	3.2497	14.2657
O	0.1816	2.1400	11.5137	0.1947	0.4007	9.4955	0.1760	2.1508	11.4925

O	3.2676	2.1403	11.5147	3.2849	0.4013	9.4940	3.2647	2.1510	11.4921
O	6.3584	2.1327	11.5224	6.3760	0.4022	9.4911	6.3552	2.1482	11.4926
O	0.1894	0.4104	9.4886	0.4299	4.1346	9.7281	0.1974	0.3818	9.5057
O	3.2845	0.4111	9.4896	3.5160	4.1315	9.7237	3.2889	0.3822	9.5054
O	6.3723	0.4130	9.4818	6.6096	4.1321	9.7239	6.3778	0.3796	9.5058
O	0.4304	4.1312	9.7333	6.1292	6.3081	34.2020	0.4192	4.1277	9.7289
O	3.5140	4.1268	9.7260	9.2006	6.2640	34.2062	3.5074	4.1272	9.7287
O	6.6113	4.1268	9.7310	3.0738	6.2628	34.2250	6.5999	4.1253	9.7287
O	-0.1680	3.8369	38.2470	-0.1171	3.8375	38.2459	-0.1341	3.8576	38.2529
O	2.9271	3.8378	38.2442	2.9862	3.7708	38.3989	2.9543	3.8535	38.2502
O	6.0089	3.8416	38.2501	5.9899	3.8765	38.2467	6.0316	3.8615	38.2504
O	0.0123	0.1754	38.4135	-0.0311	0.1528	38.3756	-0.0032	0.1463	38.3771
O	3.1050	0.1723	38.4132	6.1777	0.1641	38.2822	3.0842	0.1452	38.3789
O	6.1983	0.1764	38.4148	-0.1458	1.9082	36.3833	6.1772	0.1480	38.3772
O	-0.1164	1.9212	36.3328	6.1129	1.9164	36.3678	-0.1243	1.9532	36.3903
O	2.9737	1.9212	36.3313	2.7272	1.3729	35.1675	2.9305	1.9307	36.3908
O	6.0696	1.9241	36.3322	3.3809	0.6002	37.9332	6.0688	1.9346	36.3942
Ru	0.0000	3.1961	22.6081	0.0000	3.1961	22.6081	0.0000	3.1961	22.6081
Ru	3.0900	3.1961	22.6081	3.0900	3.1961	22.6081	3.0900	3.1961	22.6081
Ru	6.1800	3.1961	22.6081	6.1800	3.1961	22.6081	6.1800	3.1961	22.6081
Ru	0.0000	0.0000	25.8042	0.0000	0.0000	25.8042	0.0000	0.0000	25.8042
Ru	3.0900	0.0000	25.8042	3.0900	0.0000	25.8042	3.0900	0.0000	25.8042
Ru	6.1800	0.0000	25.8042	6.1800	0.0000	25.8042	6.1800	0.0000	25.8042
Ru	1.5450	0.0000	22.6081	1.5450	0.0000	22.6081	1.5450	0.0000	22.6081
Ru	4.6350	0.0000	22.6081	4.6350	0.0000	22.6081	4.6350	0.0000	22.6081
Ru	7.7250	0.0000	22.6081	7.7250	0.0000	22.6081	7.7250	0.0000	22.6081
Ru	1.5450	3.1961	25.8042	1.5450	3.1961	25.8042	1.5450	3.1961	25.8042
Ru	4.6350	3.1961	25.8042	4.6350	3.1961	25.8042	4.6350	3.1961	25.8042
Ru	7.7250	3.1961	25.8042	7.7250	3.1961	25.8042	7.7250	3.1961	25.8042
Ru	0.0558	3.2114	15.9770	0.0566	3.2135	15.9760	0.0574	3.2215	15.9804
Ru	3.1458	3.2108	15.9778	3.1467	3.2134	15.9765	3.1472	3.2212	15.9782
Ru	6.2358	3.2103	15.9746	6.2361	3.2129	15.9747	6.2369	3.2214	15.9802
Ru	3.0505	3.1818	29.0017	3.0486	3.1777	28.9771	3.0373	3.1779	28.9956
Ru	6.1407	3.1827	29.0003	6.1374	3.1794	28.9938	6.1552	3.1789	29.0003
Ru	9.2302	3.1830	29.0008	9.2329	3.1806	28.9964	9.2302	3.1794	29.0174
Ru	1.5833	3.2127	19.3540	1.5850	3.2135	19.3541	1.5890	3.2217	19.3555
Ru	4.6744	3.2135	19.3529	4.6777	3.2136	19.3534	4.6798	3.2216	19.3559
Ru	7.7630	3.2138	19.3526	7.7658	3.2136	19.3529	7.7701	3.2216	19.3553
Ru	1.4864	3.1948	32.2715	1.5283	3.2059	32.2512	1.5219	3.1715	32.3218
Ru	4.5823	3.1955	32.2719	4.5497	3.1984	32.2456	4.5746	3.1763	32.2222
Ru	7.6670	3.1941	32.2729	7.6716	3.1895	32.2415	7.6563	3.1710	32.3253
Ru	0.0379	0.0159	19.4129	0.0405	0.0167	19.4169	0.0442	0.0249	19.4225
Ru	3.1283	0.0161	19.4135	3.1312	0.0168	19.4171	3.1340	0.0251	19.4251
Ru	6.2180	0.0168	19.4119	6.2219	0.0170	19.4157	6.2243	0.0249	19.4229

Ru	3.0278	6.3865	32.4621	3.0284	-0.0003	32.4592	3.0863	6.3681	32.2577
Ru	6.1178	6.3858	32.4637	6.1112	-0.0193	32.4872	6.0784	6.3659	32.2568
Ru	9.2077	6.3851	32.4647	9.2137	-0.0025	32.4929	9.2172	6.3640	32.6004
Ru	1.6020	0.0175	16.1446	1.6047	0.0187	16.1478	1.6132	0.0225	16.1601
Ru	4.6878	0.0168	16.1439	4.6905	0.0190	16.1476	4.6888	0.0221	16.1592
Ru	7.7828	0.0173	16.1450	7.7854	0.0188	16.1474	7.7828	0.0227	16.1609
Ru	1.5023	6.3782	29.0722	1.4972	6.3745	29.0744	1.4301	6.3769	29.0712
Ru	4.5937	6.3785	29.0720	4.5990	6.3746	29.0694	4.5968	6.3754	29.0108
Ru	7.6835	6.3790	29.0725	7.6856	6.3780	29.0841	7.7654	6.3750	29.0661