Predicted Electrocatalysts Properties on Metal Insulator $MoTe_2$ for HER, and ORR Application in Fuel Cell

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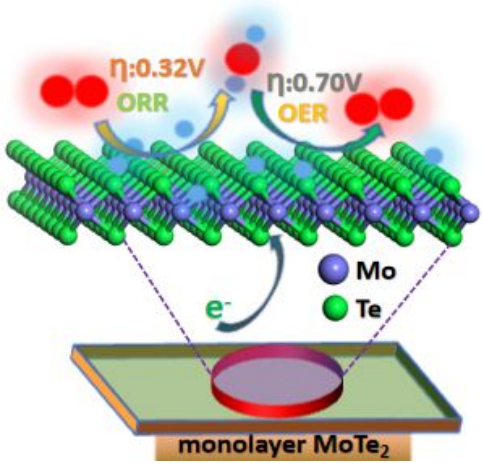
Graphical abstract



We used the theoretical model proposed by Nørskov and co-workers to calculate the formation energies of the four electron transfer step for ORR reactions. The Gibbs free energy is defined as G=E+H+ZPE-TS, it is difficult to obtain the binding energy of intermediate species under experimental conditions in the solution, thus we reference the free energy of O_2 (g) and H_2(g) and H_2O(l) to deduce the binding energy of each intermediates. The entire ORR process can be defined as follows: $O_2(g)+4(H^++e^-)\rightarrow 2H_2O(l)$ and contains four elementary steps:

(1) $O_2(g)+H^++e^-\rightarrow *OOH$

(2) $*OOH+H^++e^-\rightarrow *O+H_2O$

(3) $*O+H^++e^-\rightarrow *OH$

(4) $*OH+H^++e^-\rightarrow H_2O$

where * denotes active state, l and g represent liquid and gas phases, respectively.

Total reaction: $O_2(g)+4(H^++e^-)\rightarrow 2H_2O(l)$

$$\Delta G_{H_2O}(l) = \Delta G\{2H_2O(l) - O_2(g) - 2H_2(g)\} = -4.92\,eV \quad (1)$$

$$\Delta G_{*OOH} = \Delta G\left\{*O_2(g) + \frac{1}{2}H_2(g) \rightarrow *OOH\right\} = G_{*OOH} - G_{O_2} - \frac{1}{2}G_{H_2} - G_{substrate} \quad (2)$$

$$\Delta G_{*O} = \Delta G\left\{*O + H_2O(l) - *OOH - \frac{1}{2}H_2(g)\right\} = G_{*O} + G_{H_2O} - G_{*O} - \frac{1}{2}G_{H_2} - G_{substrate} \quad (3)$$

$$\Delta G_{*OH} = \Delta G\left\{ *OH - *O - \frac{1}{2}H_2(g) \right\}$$
$$= G_{*OH} - G_{*O} - \frac{1}{2}G_{H_2} - G_{substrate} \quad (4)$$

$$\Delta G_{*H_2O} = \Delta G\left\{ *H_2O - *OH - \frac{1}{2}H_2(g) \right\}$$
$$= G_{*H_2O} - G_{*OH} - \frac{1}{2}G_{H_2} - G_{substrate} \quad (5)$$

The reaction free energy of each elementary reaction step for electrochemical oxygen reduction can be defined as the difference between two adjacent steps, shown as follow:

$$\Delta G_1 = \Delta G_{*OOH} - 4.92 \quad (6)$$

$$\Delta G_2 = \Delta G_{*O} - \Delta G_{*OOH} \quad (7)$$

$$\Delta G_3 = \Delta G_{*OH} - \Delta G_{*O} \quad (8)$$

$$\Delta G_4 = -\Delta G_{*OH} \quad (9)$$

$$\Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 = -4.92$$

Thus, the onset electrode potential of the whole process is $U^{ORR}=-\max\{\Delta G_1, \Delta G_2, \Delta G_3, \Delta G_4\}/e$

For the association mechanism, the limiting potential of U_n(n=1, 2, 3, 4) defined as $-\Delta G_n/e$ was induced to estimate the thermodynamic limiting of each step,

$$eU_1 = 4.92 - \Delta G_{*OOH} \quad (10)$$

$$eU_2 = \Delta G_{*OOH} - \Delta G_{*O} \quad (11)$$

$$eU_3 = \Delta G_{*O} - \Delta G_{*OH} \quad (12)$$

$$eU_4 = \Delta G_{*OH} \quad (13)$$

After substituting $\Delta G_{(*OH)}$ for $\Delta G_{(*OOH)}$ and $\Delta G(O*)$ via the linear fitted equation of $\Delta G_{(*OOH)} = 0.53\Delta G_{(*OH)} + 1.24$, and $\Delta G_{(*O)} = 1.27\Delta G_{(*OH)} + 1.66$, we can obtain the limiting potential as a function of $\Delta G_{(*OH)}$.

Ui as below

$$eU_1 = 4.92 - 0.53\Delta G_{(*OH)} - 1.24 = -0.53\Delta G_{(*OH)} + 3.68 \quad (14)$$

$$eU_2 = 0.53\Delta G_{(*OH)} + 1.24 - 1.27\Delta G_{(*OH)} - 1.66 = -0.74\Delta G_{(*OH)} - 0.42 \quad (15)$$

$$eU_3 = 1.27\Delta G_{(*OH)} + 1.66 - \Delta G_{*OH} = 0.27\Delta G_{(*OH)} + 1.66 \quad (16)$$

$$eU_4 = \Delta G_{*OH} \quad (17)$$

The standard equations of thermodynamic relation states as follow:

$\Delta G=\Delta E+\Delta H+\Delta ZPE-T\Delta S$, (1)

At room temperatures (under 298.15K) and constant pressure (101,325 Pa), it can be expressed in terms of ΔE_{DFT} from DFT calculations and the enthalpy depend on heat capacity, $\Delta H= \int C_P dT$. In

addition, the entropy term can be obtained from as the sum of the translational, rotational, vibrational, and electronic contributions as to:

$S=S_t+S_r+S_v+S_e$ (2)

The intrinsic zero point energy (ZPE) and Van der Waals interactions between atoms and molecules are employed DFT-D3 to corrected,

Here, some approximations can be applied in entropy term:

At the fundamental electronic level: $S_e \approx 0$

therefore: $S=S_t+S_r+S_v$ (3)

For solids and adsorbates, both $S_t \approx 0$ and $S_r \approx 0$, and therefore: $S=S_v$

Entropy correction:

$$S_{vib}(T) = R\sum_i \left\{ \frac{h\nu_i}{kT} \frac{e^{-\frac{h\nu_i}{kT}}}{1-e^{-\frac{h\nu_i}{kT}}} - In\left[1-e^{-\frac{h\nu_i}{kT}}\right] \right\} \quad (4)$$

Finally obtain:

$\Delta G=\Delta E+\Delta(H_0+\int C_P dT)+\Delta ZPE-T\Delta(S_t+S_r+S_v+S_e)S+neU+\Delta GpH.$ (5)

The reaction free energy for each elementary step can be expressed as a function of the applied potential U and the binding energy of the ΔG_{OH*}. In this regard, we consider the possibility that the reaction follows reaction mechanism, where the nitrogen molecules are hydrogenated by protons, (* represent activation state):

Figures:

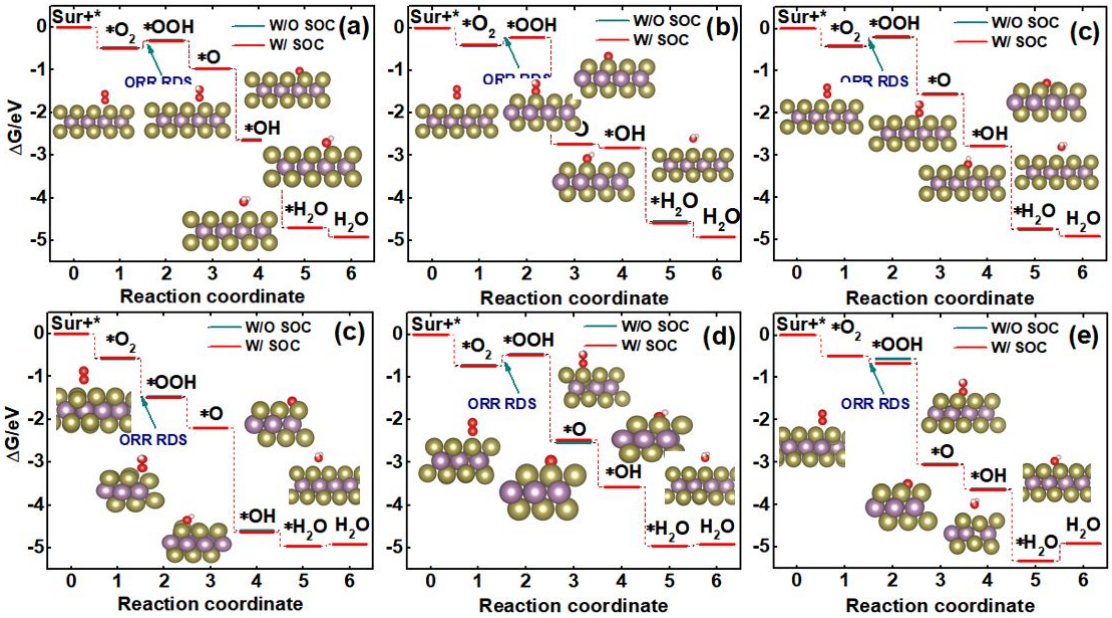


Figure S1 Gibbs free energy (ΔG) diagrams for all intermediates during ORR process, the rate-determining step with are also highlighted with arrows. (a) 2H-$MoTe_2$@α, (b) 2H-$MoTe_2$@β, (c) 2H-$MoTe_2$@γ, (d) 1T-$MoTe_2$@α, (e) 1T-$MoTe_2$@β, (f) 1T-$MoTe_2$@γ adsorption sites, respectively.

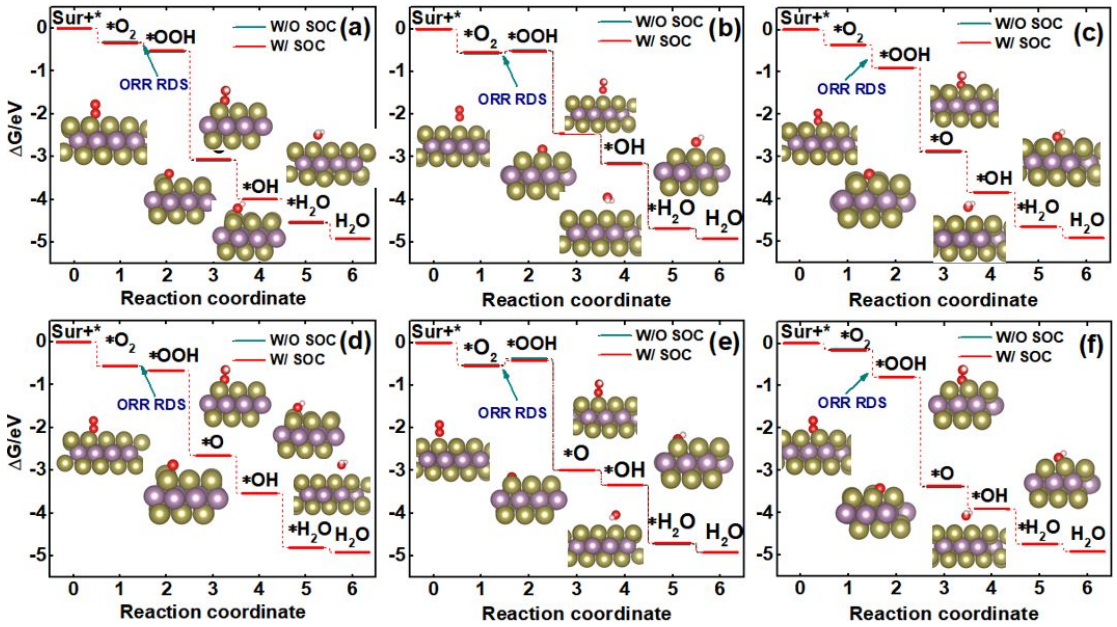


Figure S2 Gibbs free energy (ΔG) diagrams for all intermediates during ORR process, the rate-determining step with are also highlighted with arrows. (a) 1T′-$MoTe_2$@α, (b) 1T′-$MoTe_2$@β, (c) 1T′-$MoTe_2$@γ, (d) 1T′-$MoTe_2$@α′, (e) 1T′-$MoTe_2$@β′, (f) 1T′-$MoTe_2$@γ′ adsorption sites, respectively.

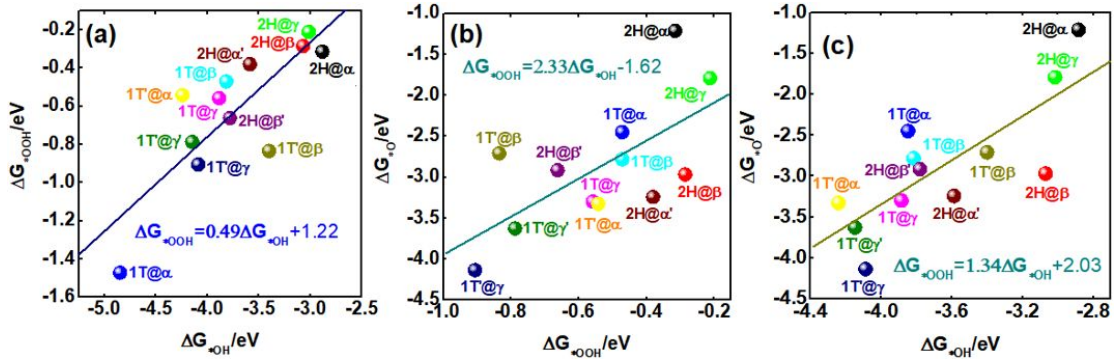
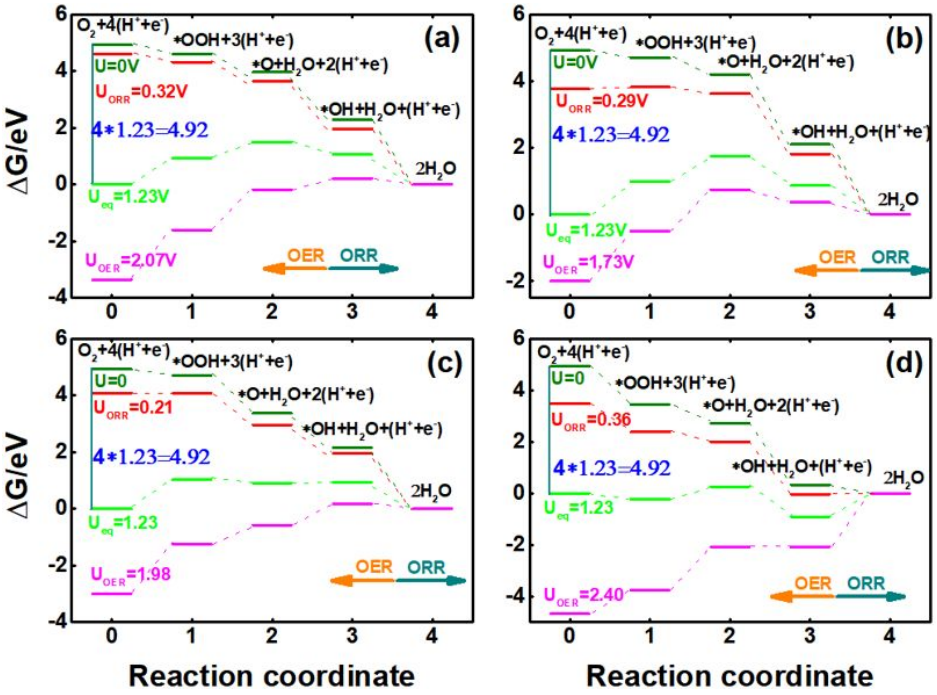


Figure S3 Linear relationships of intermediate species between binding energies without spin-orbit coupling (a) ΔG_{*OH} vs ΔG_{*OOH}; (b) ΔG_{*OOH} vs ΔG_{*O}, and ΔG_{*OH} vs ΔG_{*O}, respectively.



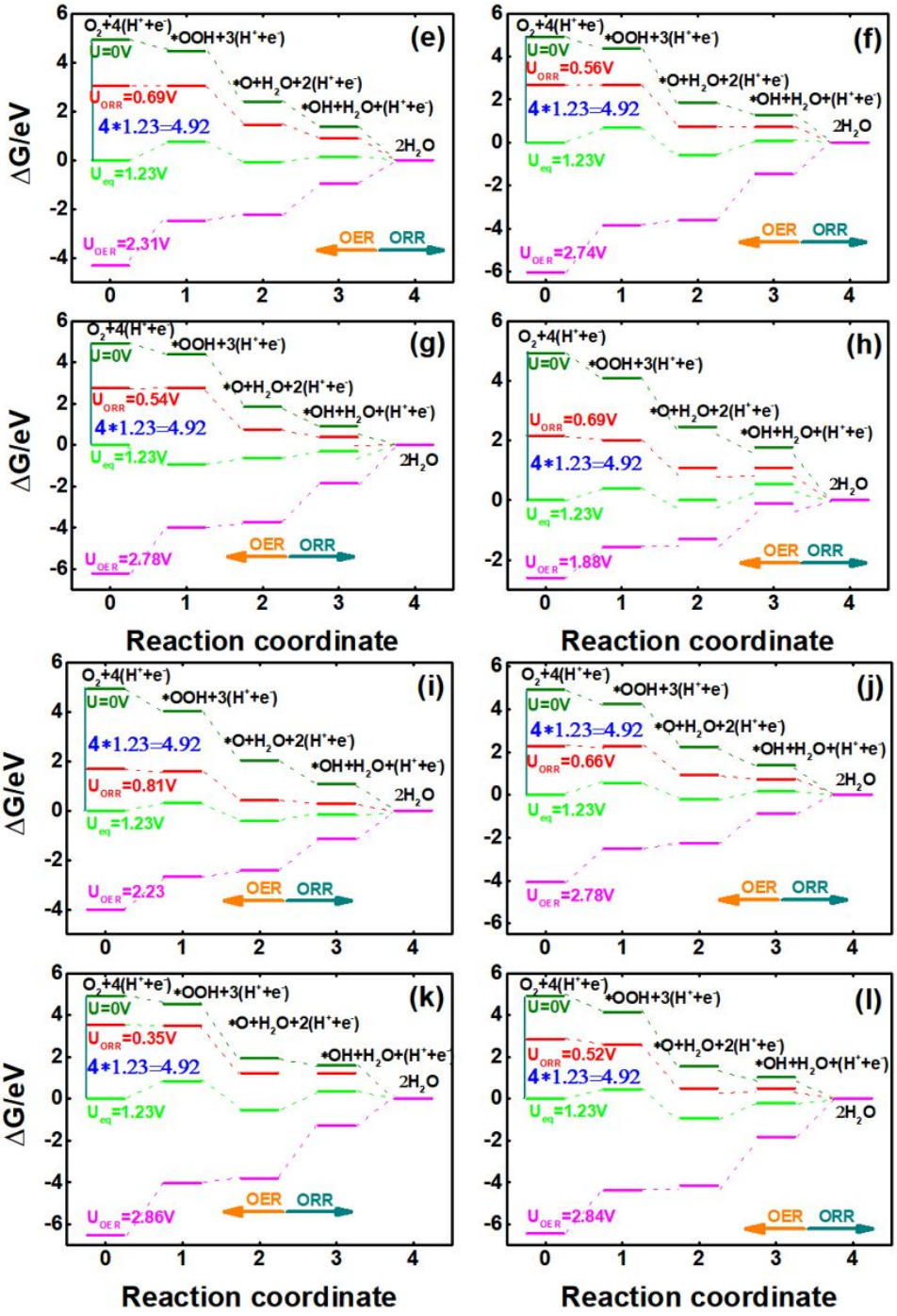


Figure.S4 Gibbs free energy diagrams without Spin orbit coupling calculations for the ORR on metal insulator monolayer $MoTe_2$ catalysts under an applied potential: reduction potential for $\Delta\Delta G_{max}$ and equilibrium potential (U=1.23V) in acidic condition (pH=0). (a) 2H-$MoTe_2$@α, (b) 2H-$MoTe_2$@β, (c) 2H-$MoTe_2$@γ, (d) 1T-$MoTe_2$@α, (e) 1T-$MoTe_2$@β, (f) 1T-$MoTe_2$@γ, (g) 1T′-$MoTe_2$@α, (h) 1T′-$MoTe_2$@β, (h) 1T′-$MoTe_2$@γ, (i) 1T″-$MoTe_2$@α′, (j) 1T″-$MoTe_2$@β′,(k) 1T″-$MoTe_2$@γ′,(l) 1T′-$MoTe_2$@β′, respectively.

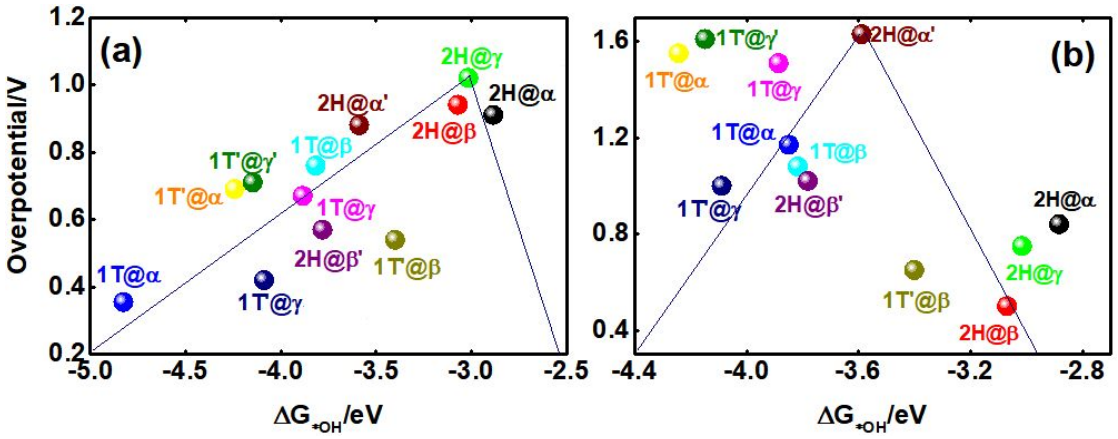


Figure S5. Volcano plot of overpotential for the ORR (a) and OER (b), the binding energies were obtained without spin-orbit coupling, respectively.

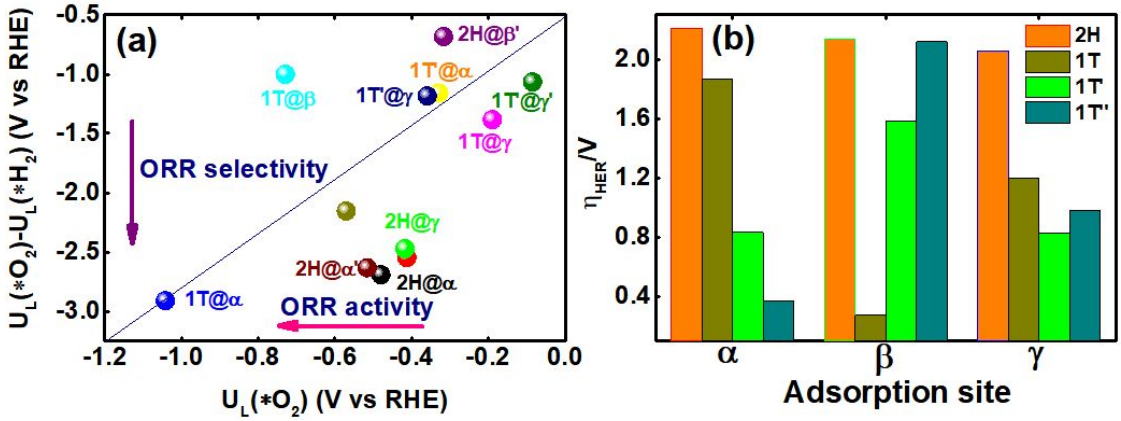


Figure S6.The activity selectivity between HER and ORR for each active site (b) the overpotential on the different adsorption sites of HER, all the binding energies without spin-orbit coupling calculations.

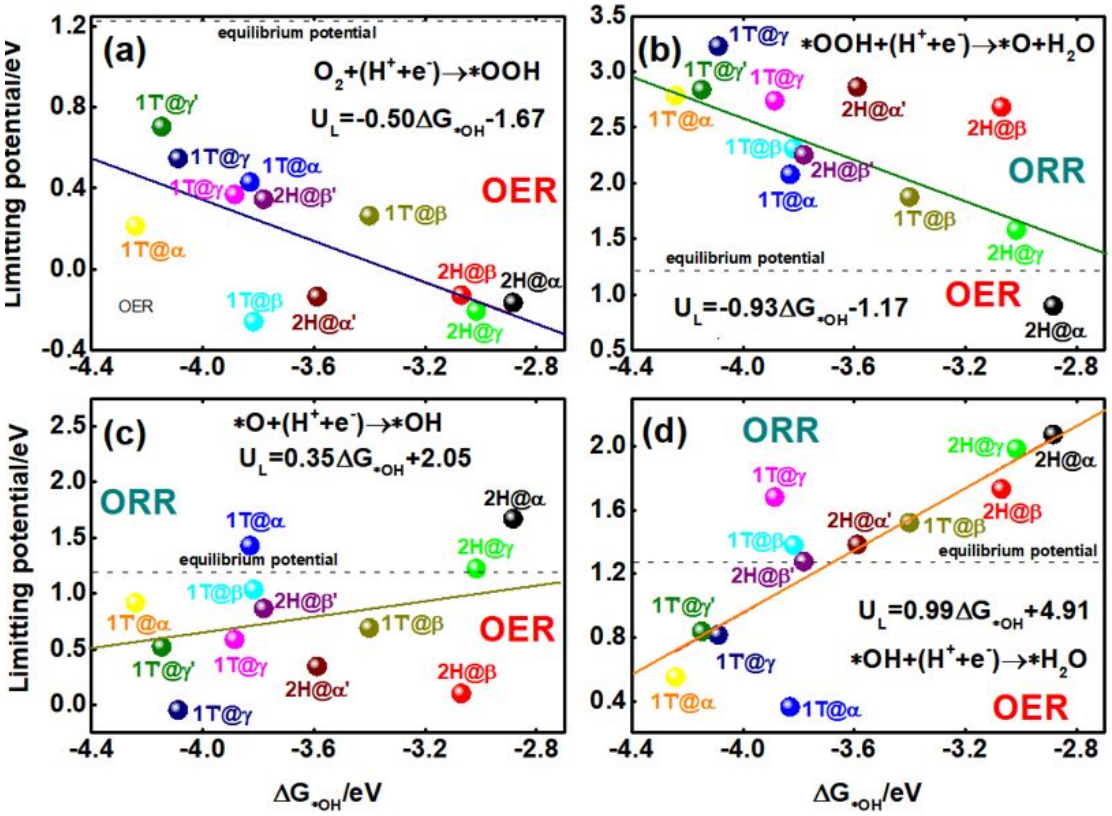


Figure S7. Activity prediction of the thermodynamical limiting potential for oxygen reduction to H_2O using ΔG_{*OH},

without spin-orbit coupling calculations, which can be obtained from the negative of the change in free energy (-ΔG) for the different reaction steps at the equilibrium potential (U=1.23) as a function of the ΔG_{*OH}, it is usually as a descriptor of the catalytic efficiency for 4e -ORR.

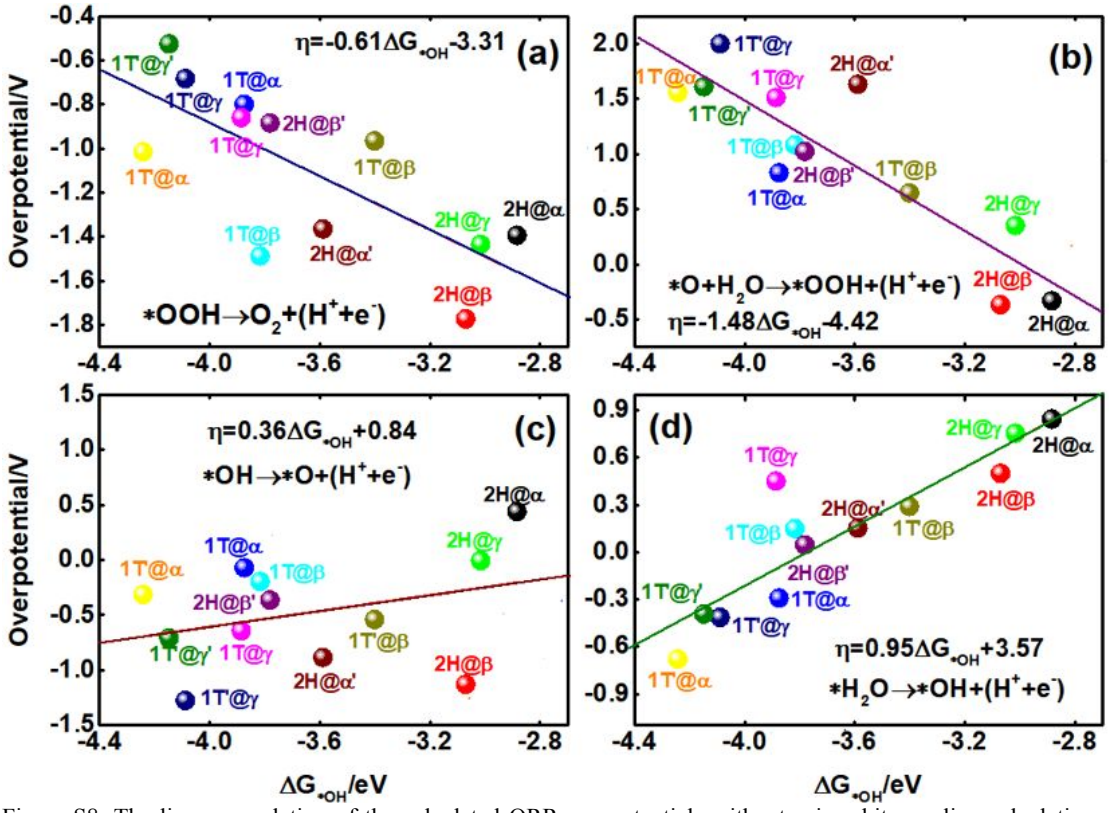


Figure S8. The linear correlation of the calculated ORR overpotentials without spin-orbit coupling calculations, and compare to the standard hydrogen electrode (SHE) vs. ΔG_{*OH} on different adsorption sites for various $MoTe_2$ phase.

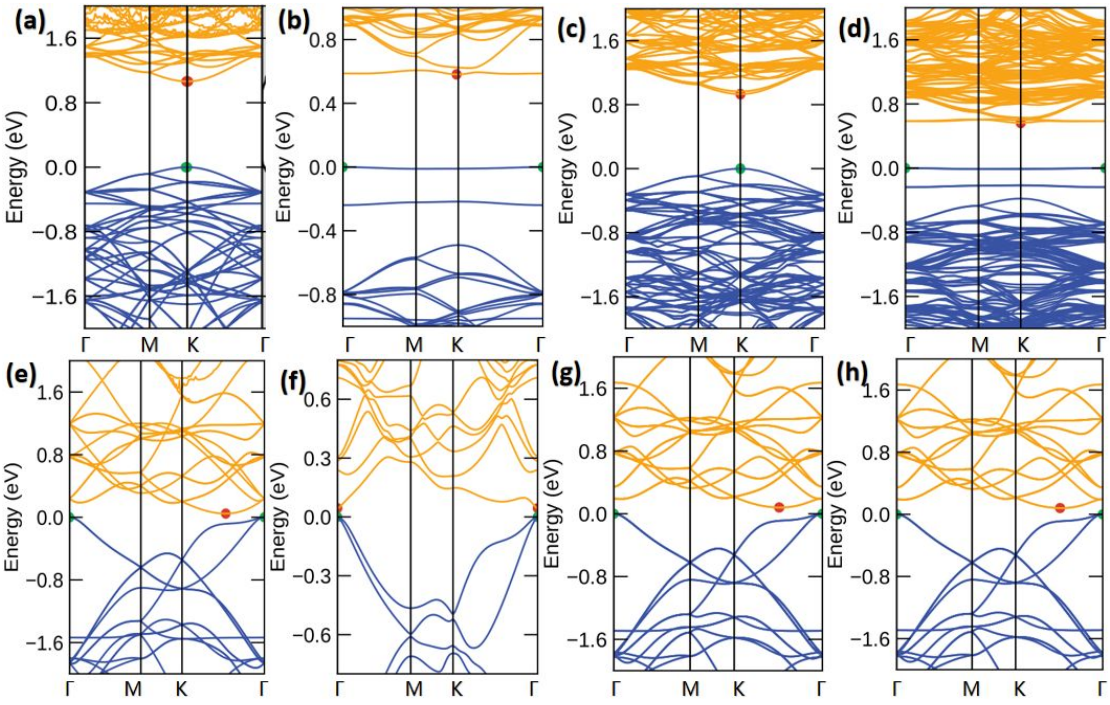


Figure S9. Electronic band structure for metal insulator $MoTe_2$ phase of (a-b) bulk surface, and O_2 adsorption configuration phase, (c-d) bulk surface, and O_2 adsorption configuration of 2H-$MoTe_2$ phase with spin orbit coupling hybrid PBE functional calculations. (e-f) bulk surface, and O_2 adsorbed configuration phase, (g-h) bulk surface, and O_2 adsorption configuration of 1T-$MoTe_2$ phase with spin orbit coupling hybrid PBE functional

calculations. The Fermi level is set to zero.

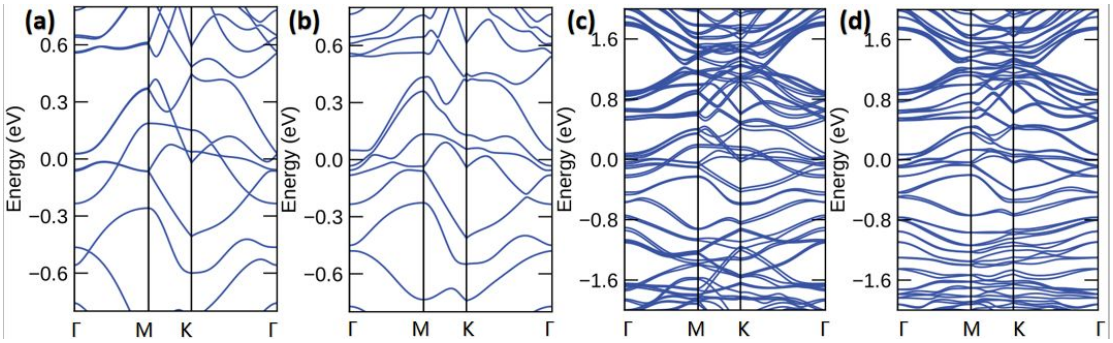


Figure S10. Electronic band structure for metal insulator 1T′-$MoTe_2$ phase of (a-b) bulk surface, and O_2 adsorption configuration phase with spin orbit coupling hybrid PBE functional calculations, respectively. (c-d) bulk surface, and O_2 adsorption configuration of 1T′-$MoTe_2$ phase with spin orbit coupling hybrid PBE functional calculations, respectively. Fermi level is set to zero.

Table S1. Gibbs free energies at 298.15 K (ZPE, H and TS corrections applied), in eV, corresponding to the each species along the O_2 conversion into water catalysed by the $MoTe_2$ different phase surfaces. G(T)=ZPE+H-TS, G=E+G(T), here G(T) is VASPKIT Gibbs corrections applied value, E is total energy from DFT calculation within D3 corrections applied.

2H	-288.54						1T	-154.41					
O_2	E	G	G(T)	ZPE	H	TS	O_2	E	G	G(T)	ZPE	H	TS
α	-298.23	-298.19	0.04	0.11	0.06	0.13	α	-164.68	-164.62	0.06	0.14	0.08	0.16
β	-298.20	-298.12	0.07	0.10	0.03	0.07	β	-164.36	-164.31	0.05	0.11	0.05	0.11
γ	-298.20	-298.17	0.03	0.12	0.08	0.17	γ	-163.78	-163.77	0.02	0.10	0.07	0.16
OOH							OOH						
α	-301.78	-301.45	0.33	0.39	0.05	0.11	α	-168.81	-168.47	0.35	0.41	0.07	0.13
β	-301.68	-301.37	0.32	0.33	0.07	0.08	β	-167.80	-167.47	0.33	0.37	0.04	0.08
γ	-301.69	-301.34	0.34	0.41	0.07	0.13	γ	-167.97	-167.55	0.41	0.44	0.05	0.08
O							O						
α	-291.63	-291.63	0.00	0.01	0.01	0.03	α	-158.74	-158.73	0.01	0.01	0.01	0.02
β	-291.41	-291.39	0.02	0.06	0.04	0.08	β	-159.11	-159.07	0.04	0.04	0.00	0.00
γ	-292.22	-292.21	0.01	0.05	0.04	0.08	γ	-159.59	-159.58	0.01	0.03	0.03	0.05
OH							OH						
α	-296.95	-296.72	0.23	0.29	0.06	0.11	α	-164.83	-164.55	0.28	0.32	0.05	0.09
β	-297.15	-296.91	0.24	0.28	0.04	0.08	β	-163.81	-163.52	0.29	0.32	0.04	0.07
γ	-297.11	-296.85	0.25	0.30	0.05	0.10	γ	-163.83	-163.59	0.24	0.29	0.05	0.11
H_2O							H_2O						
α	-302.74	-302.21	0.52	0.58	0.04	0.10	α	-168.89	-168.33	0.56	0.59	0.04	0.07
β	-302.60	-302.06	0.54	0.60	0.07	0.13	β	-168.84	-168.32	0.53	0.59	0.06	0.12
γ	-302.73	-302.25	0.48	0.59	0.08	0.19	γ	-169.23	-168.68	0.54	0.58	0.04	0.08
1T'	-155.02						1T'						
O_2	E	G	G(T)	ZPE	H	TS	O_2	E	G	G(T)	ZPE	H	TS
α	-164.89	-164.86	0.03	0.11	0.07	0.16	α'	-164.78	-164.76	0.03	0.11	0.07	0.16
β	-164.79	-164.76	0.03	0.10	0.06	0.13	β'	-164.76	-164.71	0.05	0.09	0.04	0.09

γ	-164.58	-164.54	0.05	0.12	0.06	0.14	γ'	-164.38	-164.32	0.06	0.11	0.06	0.12
OOH							OOH						
α	-168.49	-168.15	0.35	0.38	0.03	0.06	α'	-168.60	-168.27	0.34	0.40	0.07	0.13
β	-168.44	-168.12	0.32	0.39	0.07	0.14	β'	-168.31	-167.98	0.32	0.39	0.07	0.14
γ	-168.84	-168.51	0.33	0.41	0.08	0.17	γ'	-168.73	-168.39	0.34	0.41	0.08	0.15
O							O						
α	-160.21	-160.22	0.00	0.05	0.05	0.10	α'	-159.83	-159.81	0.02	0.05	0.04	0.07
β	-159.64	-159.60	0.03	0.06	0.04	0.07	β'	-160.17	-160.13	0.04	0.05	0.02	0.03
γ	-160.06	-160.03	0.04	0.06	0.03	0.05	γ'	-160.53	-160.52	0.01	0.05	0.04	0.08
OH							OH						
α	-164.83	-164.55	0.28	0.32	0.05	0.09	α'	-164.35	-164.09	0.26	0.32	0.06	0.12
β	-163.97	-163.71	0.26	0.27	0.02	0.03	β'	-164.19	-163.90	0.29	0.31	0.03	0.05
γ	-164.64	-164.40	0.25	0.30	0.05	0.11	γ'	-164.74	-164.46	0.28	0.33	0.06	0.11
H_2O							H_2O						
α	-169.06	-168.52	0.54	0.59	0.04	0.09	α'	-169.25	-168.79	0.47	0.60	0.10	0.23
β	-169.19	-168.65	0.54	0.60	0.07	0.13	β'	-169.25	-168.70	0.55	0.60	0.06	0.12
γ	-169.18	-168.63	0.55	0.58	0.04	0.07	γ'	-169.24	-168.71	0.52	0.59	0.06	0.12
SOC													
2H	-292.04						1T	-156.39					
O_2	E	G	G(T)	ZPE	H	TS	O_2	E	G	G(T)	ZPE	H	TS
α	-301.74	-301.72	0.02	0.12	0.08	0.18	α	-166.87	-166.85	0.02	0.11	0.08	0.18
β	-301.67	-301.60	0.07	0.10	0.02	0.05	β	-166.34	-166.31	0.03	0.11	0.06	0.13
γ	-301.70	-301.65	0.05	0.11	0.06	0.12	γ	-166.79	-166.75	0.04	0.10	0.04	0.10
OOH							OOH						
α	-305.29	-304.96	0.33	0.39	0.05	0.11	α	-170.82	-170.47	0.34	0.41	0.07	0.13
β	-305.04	-304.72	0.32	0.33	0.07	0.08	β	-169.79	-169.46	0.33	0.37	0.04	0.08
γ	-305.16	-304.82	0.34	0.41	0.07	0.13	γ	-169.96	-169.64	0.32	0.40	0.07	0.15
O							O						
α	-295.14	-295.14	0.00	0.01	0.01	0.03	α	-160.72	-160.72	0.00	0.01	0.01	0.02
β	-296.87	-296.85	0.02	0.06	0.04	0.08	β	-161.08	-161.79	-0.71	0.62	1.22	2.55
γ	-295.73	-295.73	0.00	0.04	0.05	0.09	γ	-161.57	-161.57	0.01	0.03	0.03	0.05
OH							OH						
α	-300.48	-300.25	0.23	0.29	0.06	0.11	α	-166.83	-166.56	0.27	0.32	0.32	0.09
β	-300.64	-300.40	0.24	0.28	0.04	0.08	β	-165.80	-165.51	0.29	0.32	0.04	0.08
γ	-300.63	-300.51	0.12	0.21	0.07	0.16	γ	-165.83	-165.58	0.25	0.29	0.05	0.10
H_2O							H_2O						
α	-306.22	-305.70	0.52	0.58	0.04	0.10	α	-170.87	-170.31	0.56	0.59	0.04	0.07
β	-306.16	-305.59	0.57	0.58	0.02	0.03	β	-170.82	-170.29	0.52	0.59	0.59	0.13
γ	-306.22	-305.75	0.48	0.59	0.08	0.19	γ	-171.22	-170.68	0.54	0.58	0.04	0.08
1T'	-157.02						1T'	-157.02					
O_2	E	G	G(T)	ZPE	H	TS	O_2	E	G	G(T)	ZPE	H	TS

α	-166.74	-166.69	0.05	0.10	0.04	0.09	α'	-166.79	-166.74	0.05	0.10	0.04	0.09
β	-166.79	-166.74	0.06	0.06	0.04	0.09	β'	-166.77	-166.73	0.04	0.10	0.04	0.04
γ	-166.59	-166.54	0.05	0.12	0.06	0.13	γ'	-166.38	-166.35	0.03	0.10	0.05	0.12
OOH							OOH						
α	-170.49	-170.14	0.35	0.38	0.03	0.06	α'	-170.61	-170.28	0.33	0.40	0.07	0.13
β	-170.44	-170.13	0.32	0.39	0.07	0.14	β'	-170.36	-170.03	0.33	0.39	0.07	0.13
γ	-170.84	-170.51	0.33	0.41	0.08	0.08	γ'	-170.73	-170.40	0.34	0.41	0.08	0.15
O							O						
α	-162.21	-162.21	0.00	0.05	0.05	0.10	α'	-161.83	-161.81	0.02	0.05	0.04	0.07
β	-161.63	-161.59	0.03	0.06	0.04	0.07	β'	-162.17	-162.13	0.04	0.05	0.02	0.03
γ	-163.05	-163.02	0.04	0.06	0.03	0.05	γ'	-162.53	-162.52	0.01	0.05	0.04	0.08
OH							OH						
α	-166.83	-166.56	0.27	0.32	0.05	0.09	α'	-166.36	-166.10	0.26	0.32	0.06	0.13
β	-165.97	-165.72	0.25	0.27	0.02	0.04	β'	-166.19	-165.90	0.29	0.31	0.03	0.05
γ	-166.64	-166.40	0.24	0.30	0.05	0.11	γ'	-166.74	-166.46	0.28	0.33	0.06	0.11
H_2O							H_2O						
α	-171.05	-170.52	0.53	0.59	0.04	0.09	α'	-171.26	-170.79	0.47	0.60	0.10	0.23
β	-171.19	-170.65	0.54	0.60	0.07	0.13	β'	-171.24	-170.67	0.57	0.61	0.05	0.10
γ	-171.18	-170.63	0.54	0.58	0.04	0.08	γ'	-171.24	-170.71	0.53	0.60	0.06	0.12

Table S2. Binding energy values of adsorbates for both HER and ORR on each adsorption site for the three different phase $MoTe_2$ structures, without and with spin-orbit coupling are all considered in this study.

W/O SOC	*H	*O_2	*OOH	*O	*OH	*H_2O	H_2O
α	2.20647	-0.48022	-0.31557	-0.9641	-2.63368	-4.70725	0.21102
β	2.06313	-0.41236	-0.23543	-2.7282	-2.82003	-4.54971	0.36856
γ	2.05338	-0.41759	-0.21212	-1.54277	-2.76576	-4.74931	0.16896
α	1.82087	-0.57850	-1.47198	-2.19956	-4.59867	-4.91827	-0.04203
β	0.88467	-0.72932	-0.47129	-2.5329	-3.56668	-4.91827	-0.02675
γ	1.11342	-0.49034	-0.5585	-3.04852	-3.63529	-5.31450	-0.39623
α	0.66948	-0.32878	-0.54230	-3.07723	-3.99245	-4.54187	0.3764
β	1.46844	-0.57060	-0.5182	-2.46065	-3.15049	-4.66904	0.24923
γ	0.68288	-0.35926	-0.90606	-2.8842	-3.83835	-4.65304	0.26523
α'	0.22925	-0.57135	-0.66237	-2.66603	-3.53117	-4.80705	0.11122
β'	2.11409	-0.53255	-0.38056	-2.99246	-3.33821	-4.71970	0.19857
γ'	0.84739	-0.13894	-0.78806	-3.37675	-3.89803	-4.73408	0.18419
W/ SOC	*H	*O_2	*OOH	*O	*OH	*H_2O	H_2O
α	2.25385	-0.50528	-0.32605	-0.9701	-2.65953	-4.69157	0.22670
β	2.068	-0.39106	-0.23125	-2.6384	-2.81242	-4.58501	0.33326
γ	2.05558	-0.40838	-0.19451	-1.55833	-2.92679	-4.74148	0.17679
α	1.80498	-0.55495	-1.49872	-2.20584	-4.63009	-4.96239	-0.04412
β	0.91314	-0.74954	-0.48729	-2.4790	-3.57660	-4.94602	-0.02775
γ	1.11602	-0.49188	-0.5662	-3.05373	-3.64990	-5.32818	-0.40991

α	0.67265	-0.33935	-0.53367	-3.06737	-3.99517	-4.53634	0.38193
β	1.46213	-0.54576	-0.5221	-2.44820	-3.15234	-4.67230	0.24597
γ	0.69955	-0.35256	-0.90081	-2.8708	-3.83426	-4.65235	0.26592
α'	0.20071	-0.55562	-0.67238	-2.66509	-3.54035	-4.80937	0.10890
β'	2.10989	-0.54035	-0.42256	-2.98914	-3.33516	-4.69069	0.22758
γ'	0.85703	-0.15891	-0.79061	-3.37116	-3.89730	-4.72658	0.19169

Table S3. Limiting potentials for the ORR and HER and $U_L(O_2)$ -$U_L(H_2)$ for as-selected adsorption site on different $MoTe_2$ phase, binding energy values of adsorbates for both *H and *O_2 on each adsorption site for the three different phase $MoTe_2$ structures, without and with spin-orbit coupling are all considered in this study.

O/W SOC	$U_L(H_2)$	$U_L(O_2)$	$U_L(O2)$-$U_L(H_2)$	W/SOC	$U_L(H_2)$	$U_L(O_2)$	$U_L(O2)$-$U_L(H_2)$
α	2.21179	-0.48022	-2.69201	α	2.23504	-0.50528	-2.74032
β	2.13546	-0.41236	-2.54782	β	2.1511	-0.26106	-2.41216
γ	2.05628	-0.41759	-2.47387	γ	2.07468	-0.40838	-2.48306
α	1.86964	-1.04188	-2.91152	α	1.85301	-1.29336	-3.14637
β	0.27274	-0.72932	-1.00206	β	1.05171	-0.74954	-1.80125
γ	1.19528	-0.18941	-1.38469	γ	1.19847	-1.19188	-2.39035
α	0.8313	-0.32878	-1.16008	α	0.84169	-0.49935	-1.34104
β	1.58524	-0.57060	-2.15584	β	1.48474	-0.54576	-2.0305
γ	0.82446	-0.35926	-1.18372	γ	0.8404	-0.35256	-1.19296
α'	0.36628	-0.31697	-0.68325	α'	2.22463	-0.55562	-2.78025
β'	2.11839	-0.51571	-2.6341	β'	1.35018	-0.54035	-1.89053
γ'	0.98022	-0.08463	-1.06485	γ'	0.99133	-0.15891	-1.15024

Table S4. Gibbs free energy profile, limiting potentials and overpotential of each elementary reaction step for the ORR with and without spin-orbit coupling calculation.

2H	**α**		**U_L**		**Overpotential**	
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.3156	-0.3261	0.3156	0.3261	**0.9144**	**0.9040**
*O	-0.9641	-0.9701	0.6485	0.6441	0.5815	0.5859
*OH	-2.6337	-2.6595	1.6696	1.6894	-0.4396	-0.4594
H2O	-4.9183	-4.9183	2.2846	2.2587	-1.0546	-1.0287
1T	α		**U_L**		**Overpotential**	
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-1.4720	-1.4987	1.4720	1.4987	-0.2420	-0.2687
*O	-2.1996	-2.2058	0.7276	0.7071	0.5024	0.5229
*OH	-4.5987	-4.6301	2.3991	2.4243	-1.1691	-1.1943
H2O	-4.9183	-4.9183	0.3196	0.2882	**0.9104**	**0.9418**
1T'	α					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				

*OOH	-0.5423	-0.5337	0.5423	0.5337	0.6877	0.6963
*O	-3.0772	-3.0674	2.5349	2.5337	-1.3049	-1.3037
*OH	-3.9925	-3.9952	0.9152	0.9278	0.3148	0.3022
H2O	-4.9183	-4.9183	0.9258	0.9231	0.3042	0.3069
1T"	α					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.6624	-0.6724	0.6624	0.6724	**0.5676**	**0.5576**
*O	-2.6660	-2.6651	2.0037	1.9927	-0.7737	-0.7627
*OH	-3.5312	-3.5404	0.8651	0.8753	0.3649	0.3547
H2O	-4.9183	-4.9183	1.3871	1.3779	-0.1571	-0.1479
2H	β					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.2354	-0.2313	0.2354	0.2313	0.9946	0.9988
*O	-2.7282	-2.6384	2.4928	2.4071	-1.2628	-1.1771
*OH	-2.8200	-2.8124	0.0918	0.1741	1.1382	1.0559
H2O	-4.9183	-4.9183	2.0982	2.1059	-0.8682	-0.8759
	β					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.4713	-0.4873	0.4713	0.4873	**0.7587**	**0.7427**
*O	**-2.5329**	**-2.4790**	2.0616	1.9917	-0.8316	-0.7617
*OH	-3.5667	-3.5766	1.0338	1.0976	0.1962	0.1324
H2O	-4.9183	-4.9183	1.3516	1.3417	-0.1216	-0.1117
1T'	β					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.5182	-0.5221	0.5182	0.5221	0.7118	0.7079
*O	-2.4607	-2.4482	1.9425	1.9261	-0.7125	-0.6961
*OH	-3.1505	-3.1523	0.6898	0.7041	0.5402	0.5259
H2O	-4.9183	-4.9183	1.7678	1.7659	-0.5378	-0.5359
1T"	β					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.3806	-0.4226	0.3806	0.4226	0.8494	0.8074
*O	-2.9925	-2.9891	2.6119	2.5666	-1.3819	-1.3366
*OH	-3.3382	-3.3352	0.3458	0.3460	0.8843	0.8840
H2O	-4.9183	-4.9183	1.5801	1.5831	-0.3501	-0.3531
2H	γ					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				

*OOH	-0.2121	-0.1945	0.2121	0.1945	1.0179	1.0355
*O	-1.5428	-1.5583	1.3307	1.3638	-0.1007	-0.1338
*OH	-2.7658	-2.9268	1.2230	1.3685	0.0070	-0.1385
H2O	-4.9183	-4.9183	2.1525	1.9915	-0.9225	-0.7615
1T	γ					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.5585	-0.5662	0.5585	0.5662	**0.6715**	**0.6638**
*O	-3.0485	-3.0537	2.4900	2.4875	-1.2600	-1.2575
*OH	-3.6353	-3.6499	0.5868	0.5962	0.6432	0.6338
H2O	-4.9183	-4.9183	1.2830	1.2684	-0.0530	-0.0384
1T'	γ					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.9061	-0.9008	0.9061	0.9008	**0.3239**	**0.3292**
*O	-2.8842	-2.8708	1.9781	1.9700	-0.7481	-0.7400
*OH	-3.8384	-3.8343	0.9542	0.9635	0.2758	0.2665
H2O	-4.9183	-4.9183	1.0799	1.0840	0.1501	0.1460
1T''	γ					
U=0	W/O SOC	W/ SOC	W/O SOC	W/ SOS	W/O SOC	W/ SOC
Sur	0.0000	0.0000				
*OOH	-0.7881	-0.7906	0.7881	0.7906	0.4419	0.4394
*O	-3.3768	-3.3712	2.5887	2.5806	-1.3587	-1.3506
*OH	-3.8980	-3.8973	0.5213	0.5261	0.7087	0.7039
H2O	-4.9183	-4.9183	1.0202	1.0210	0.2098	0.2090

Table S5 Calculated band gap and spin-orbit coupling (Δ_{SOC}) of the valence band maximum at K points for monolayer 2H-$MoTe_2$ and 1T-$MoTe_2$ for between K and Γ points with PBE without SOC and with SOC, respectively.

Methods	2H	Δ_{SOC} (eV)	1T	Δ_{SOC} (eV)
PBE W/O SOC	1.064		0.129	
PBE W/ SOC	0.932	0.132	0.167	-0.038