Analysis of Tin Oxide Supported Transition Metal Single-Atom Catalysts for Oxygen Evolution Reaction

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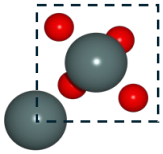
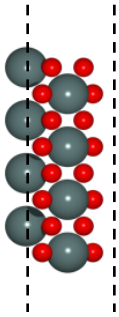
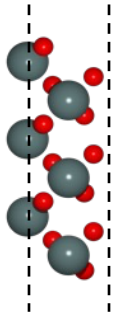
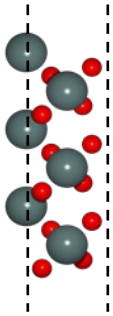
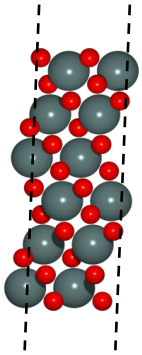
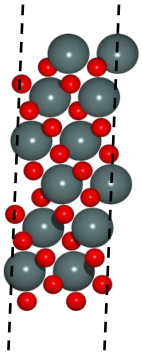
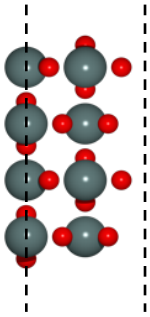
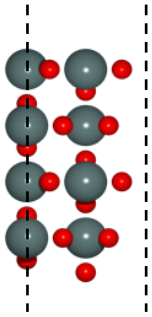
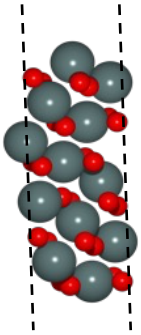
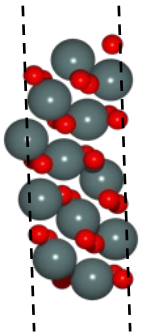
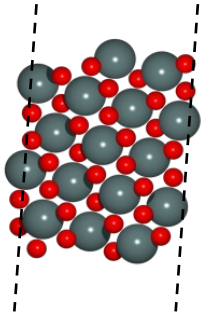
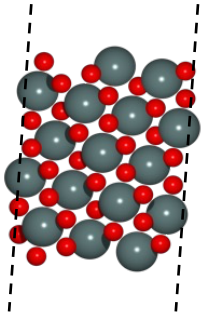
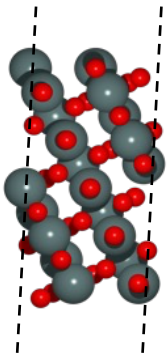
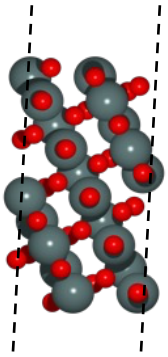
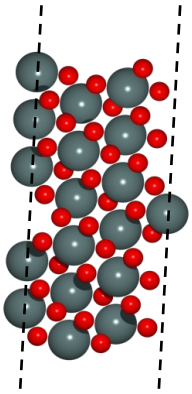
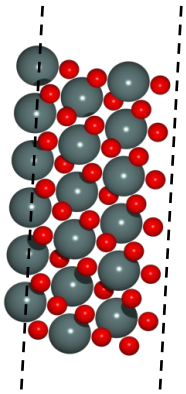
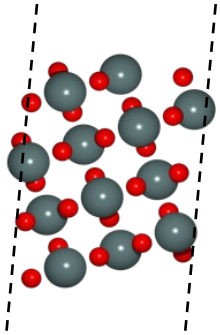
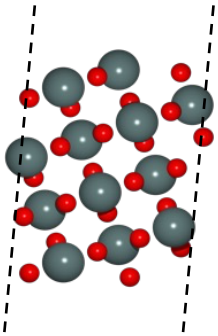
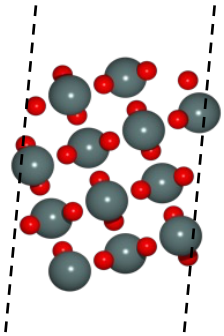
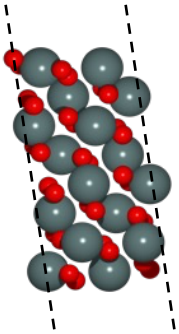
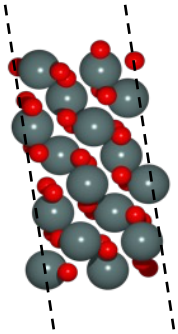
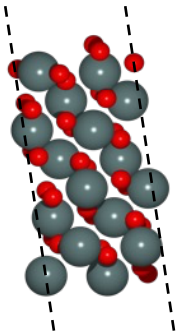
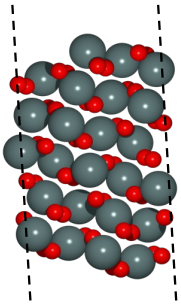
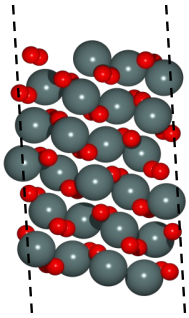
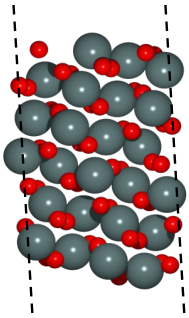
(a) SnO_2 bulk structure



(b)

Surface	Atomistic figures	
$SnO_2(001)$		
Polarity	Non-polar	
Surface energy (eV)	1.40	
$SnO_2(100)$		
Polarity	Non-polar	Polar
Surface energy (eV)	0.67	2.42
$SnO_2(101)$		
Polarity	Non-polar	Polar
Surface energy (eV)	0.99	2.58

$SnO_2(110)$		
Polarity	Non-polar	Polar
Surface energy (eV)	0.65	2.01
$SnO_2(111)$		
Polarity	Polar	Non-polar
Surface energy (eV)	1.48	1.86
$SnO_2(102)$		
Polarity	Polar	Non-polar
Surface energy (eV)	1.74	2.17
$SnO_2(112)$		
Polarity	Polar	Non-polar
Surface energy (eV)	1.60	2.02

SnO_2(201)			
Polarity	Non-polar	Polar	
Surface energy (eV)	0.99	1.63	
SnO_2(210)			
Polarity	Non-polar	Polar	Polar
Surface energy (eV)	1.16	2.36	1.51
SnO_2(211)			
Polarity	Non-polar	Polar	Polar
Surface energy (eV)	1.03	1.39	2.03
SnO_2(212)			
Polarity	Polar	Polar	Non-polar
Surface energy (eV)	1.27	1.93	1.54

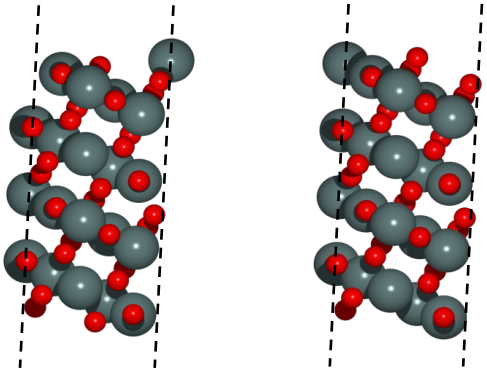
SnO_2(221)		
Polarity	Polar	Non-polar
Surface energy (eV)	1.15	1.29

Figure S1. Bulk structure and considered facets of SnO_2. (a) SnO_2 (mp-856) unit cell corresponding to tetragonal-$P4_2/mnm$ space group, (b) Side views of considered facets (up to miller index 2) of SnO_2 for the surface energy analysis. Polarity and the surface energies of the respective facets are mentioned in the same figure. Color code: dark gray – Sn, red – oxygen.

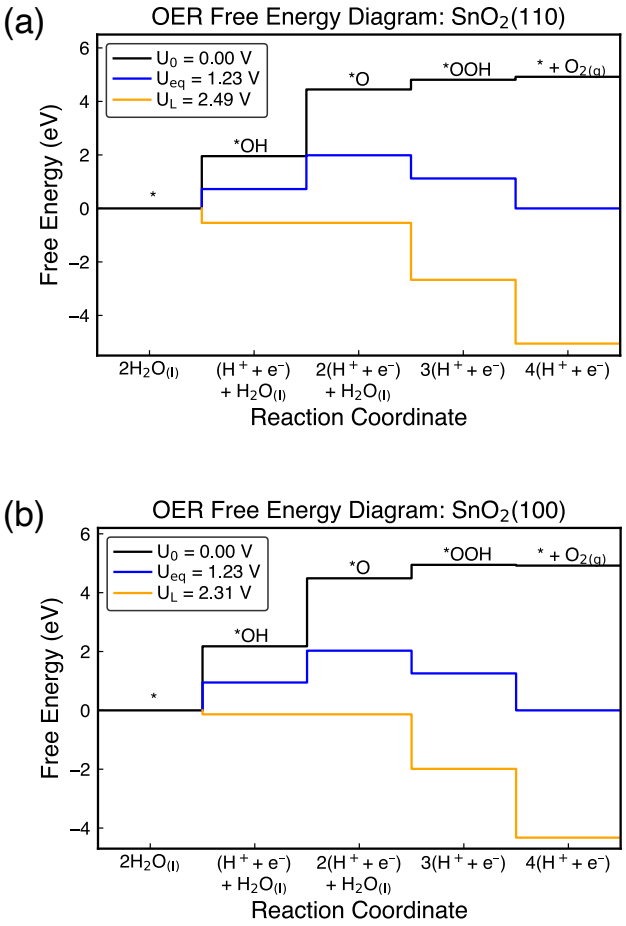


Figure S2. OER activity of pristine SnO_2(110) and SnO_2(100) facets. Free energy diagrams for (a) SnO_2(110) (b) SnO_2(100) representing the potential dependent adsorption strengths of OER intermediates at U = 0, 1.23 and limiting potential (V vs RHE).

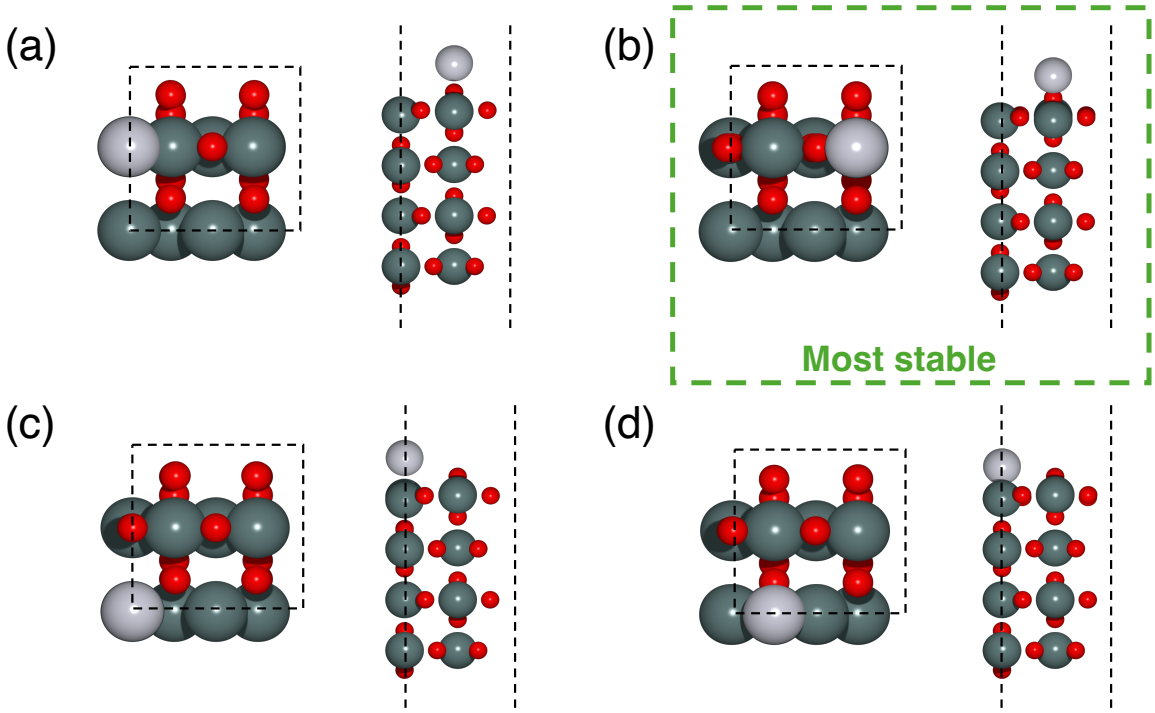


Figure S3. Considered adatom configurations for SnO_2(110). Several adsorption sites of single TM–SACs were considered as (a), (b), (c) and (d). Left – top view and right – side views were shown for each configuration. Adatom configuration shown in (b) was found to be the most stable for all TM SACs on SnO_2(110). Color code: dark gray – Sn, red – oxygen and light gray – Ag.

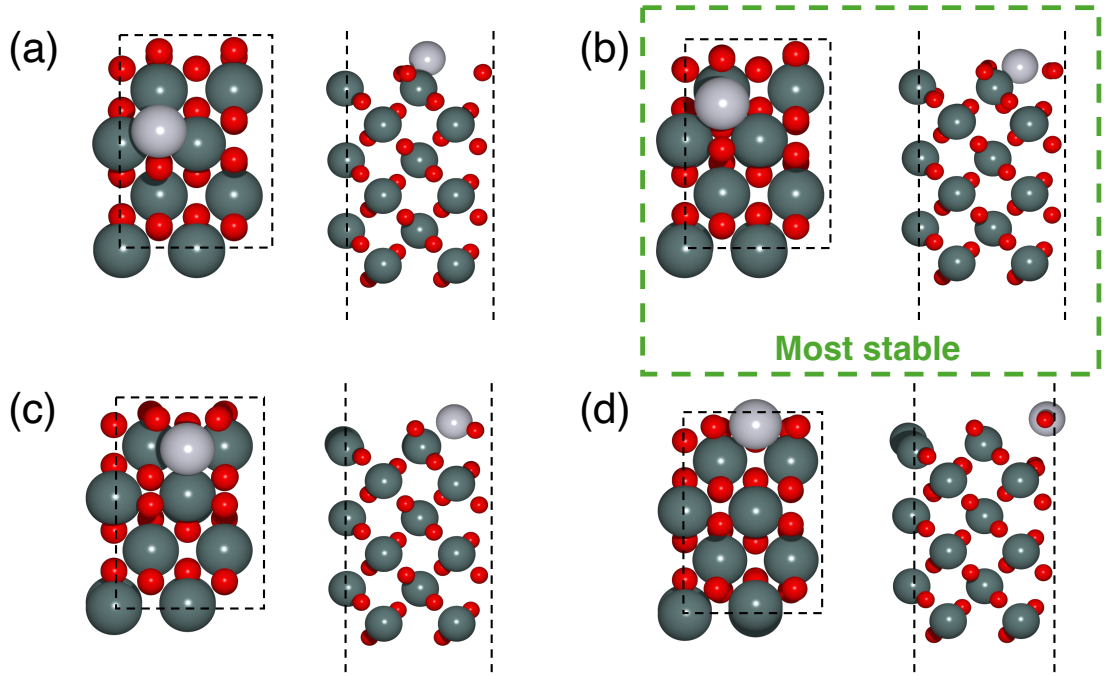


Figure S4. Considered adatom configurations for SnO_2(100). Several adsorption sites of single TM–SAC were considered as (a), (b), (c) and (d). Left – top view and right – side view were shown for each configuration. Adatom configuration shown in (b) was found to be the most stable for all TM–SACs on SnO_2(100). Color code: dark gray – Sn, red – oxygen and light gray – Ag.

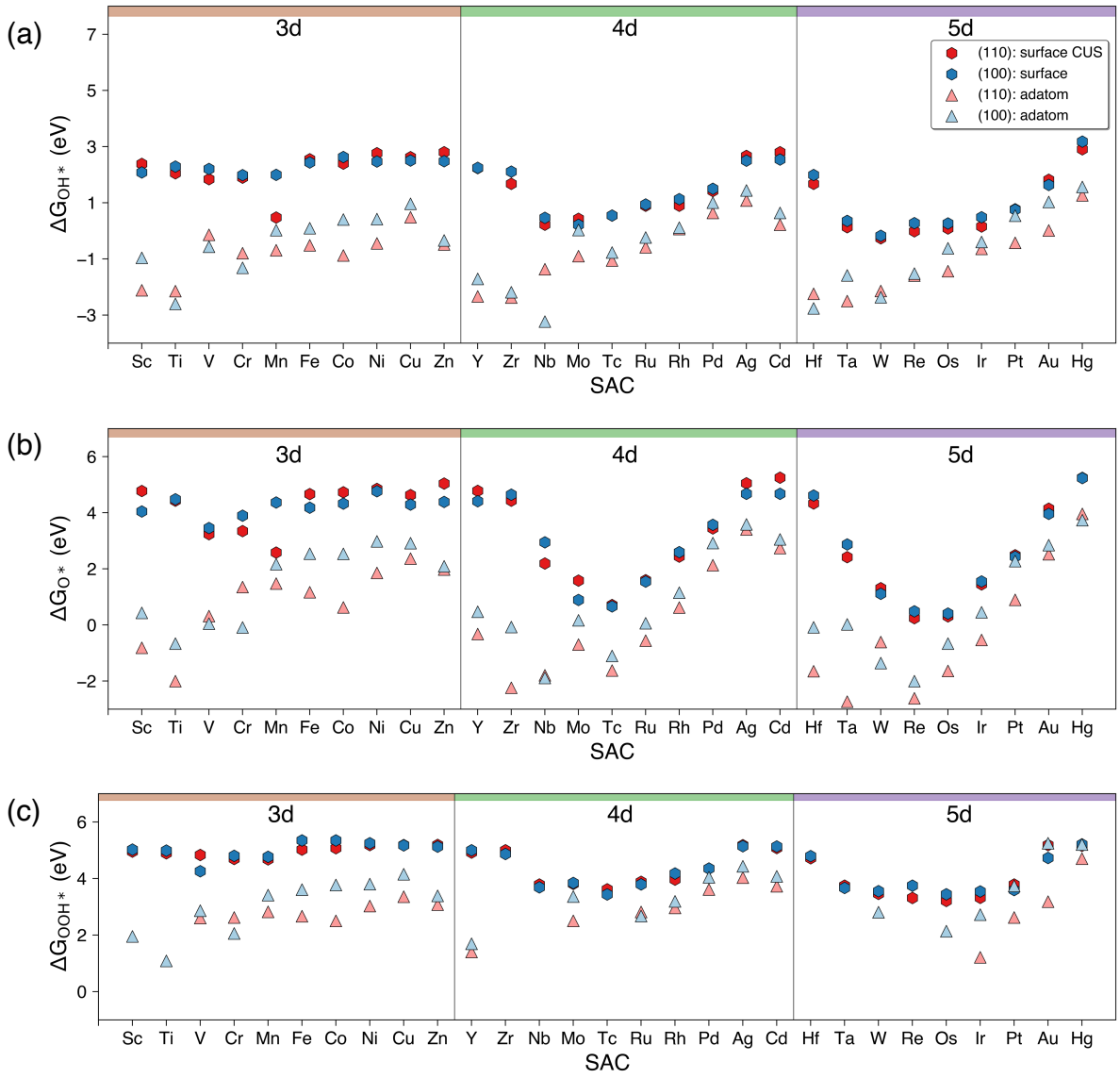


Figure S5. Adsorption energy trends of OER intermediates on SnO_2(110): surface CUS, SnO_2(100): surface, SnO_2(110): adatom and SnO_2(100): adatom configurations. Free energies of adsorption of (a) OH*, (b) O* and (c) OOH* as a function of TM–SAC. Several adatom data points of OOH* were excluded due to OOH* dissociation to OH* and O*.

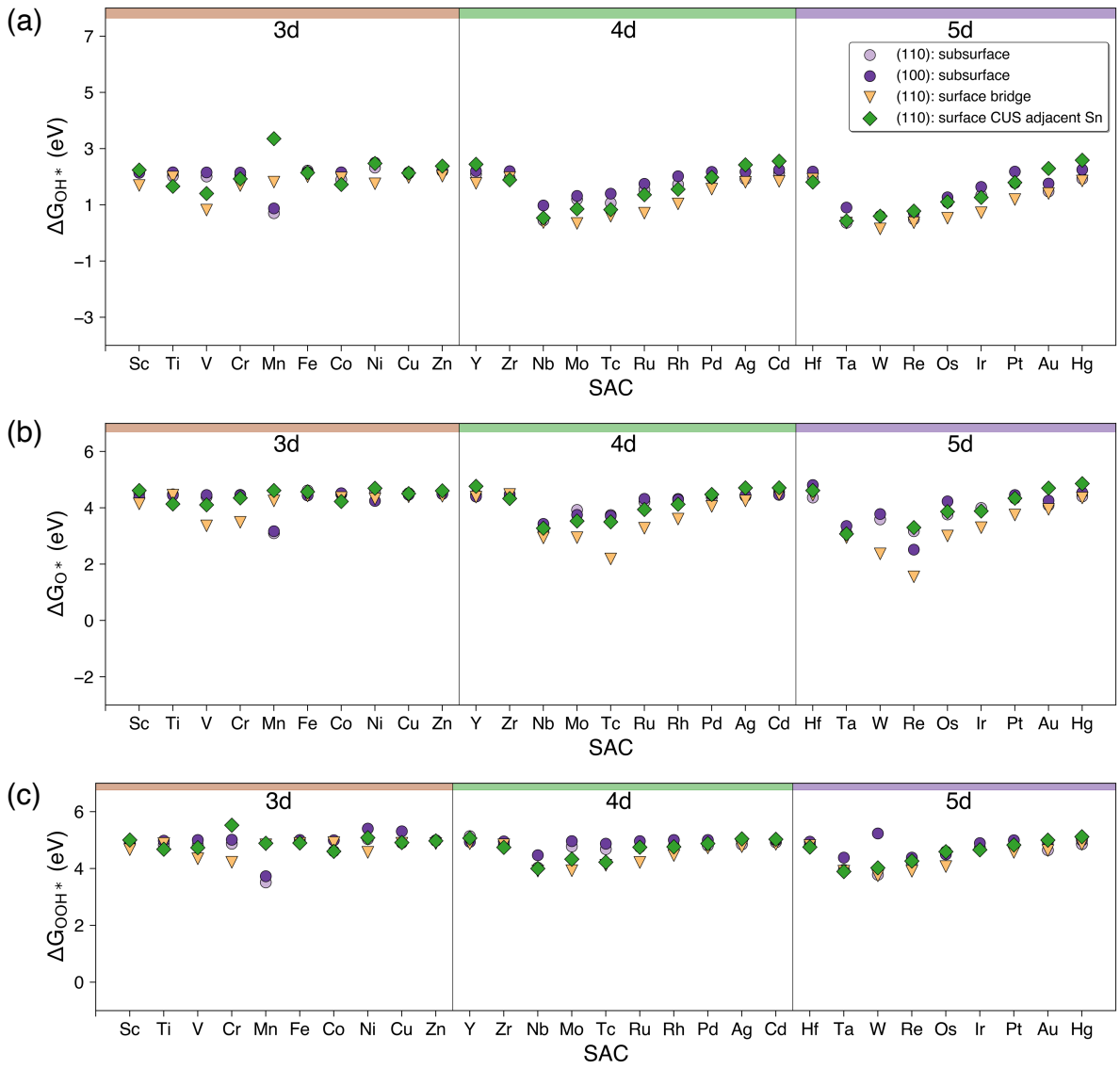
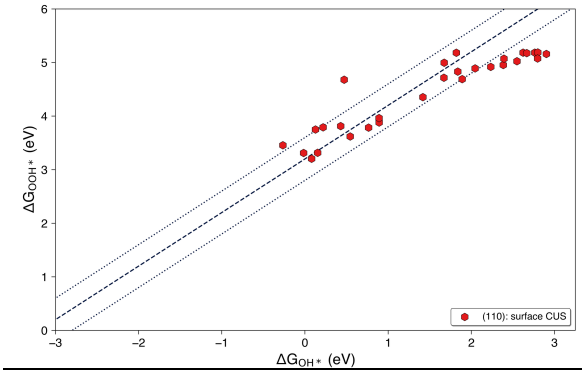


Figure S6. Adsorption energy trends of OER intermediates on surface Sn active site when the SAC is on SnO_2(110): subsurface, SnO_2(100): subsurface, SnO_2(110): surface bridge and SnO_2(110): surface CUS configurations. Free energies of adsorption of (a) OH*, (b) O* and (c) OOH* as a function of TM–SAC.

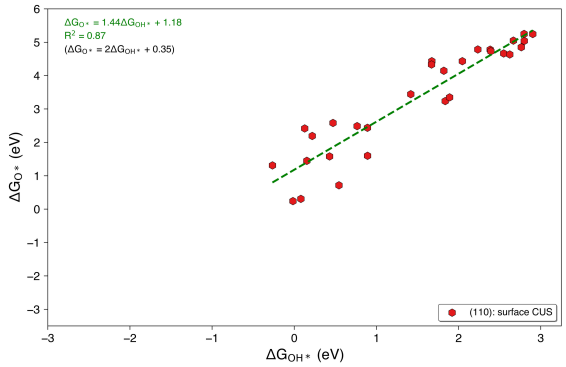
ΔG_{OOH*} vs. ΔG_{OH*}	ΔG_{O*} vs. ΔG_{OH*}

SAC configuration – (110): surface CUS | Adsorption site – TM SAC

(a)

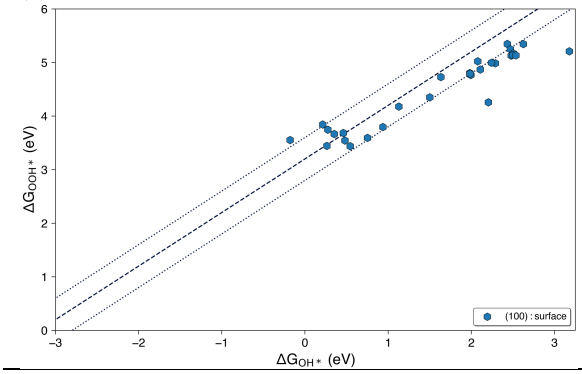


(b)

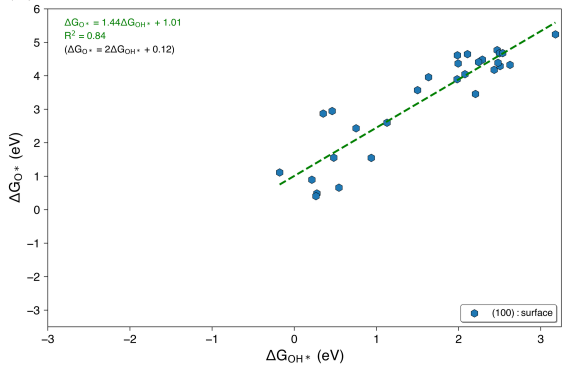


SAC configuration – (100): surface | Adsorption site – TM SAC

(c)

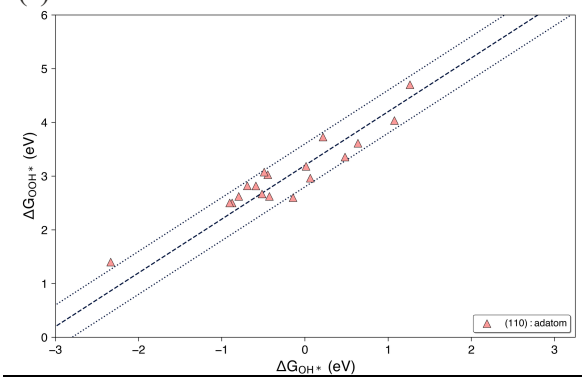


(d)

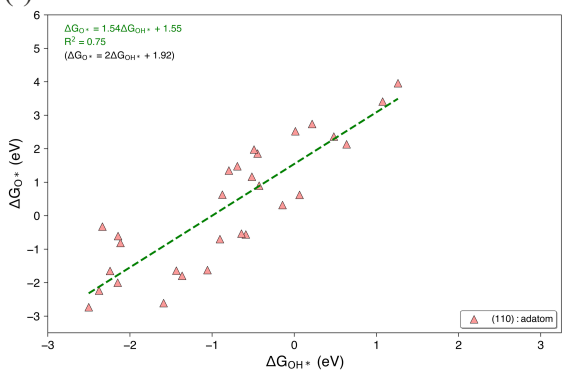


SAC configuration – (110): adatom | Adsorption site – TM SAC

(e)

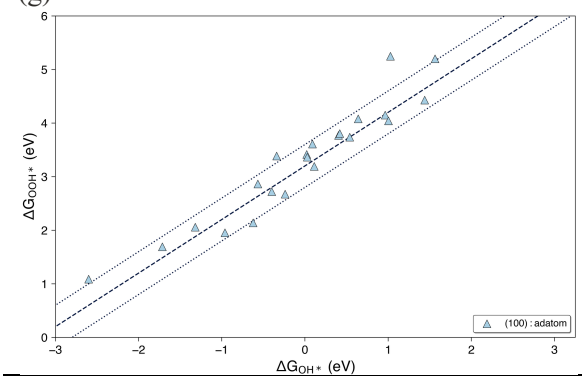


(f)

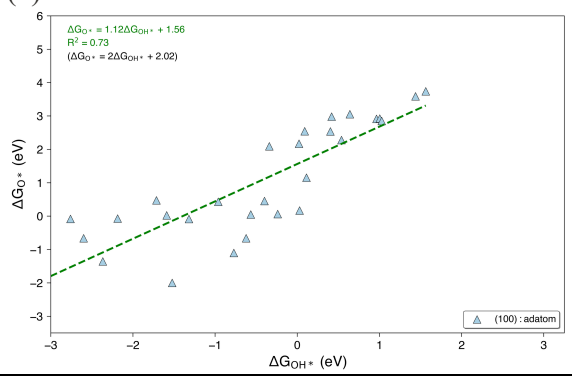


SAC configuration – (100): adatom | Adsorption site – TM SAC

(g)



(h)



SAC configuration: (110): subsurface | Adsorption site – Sn

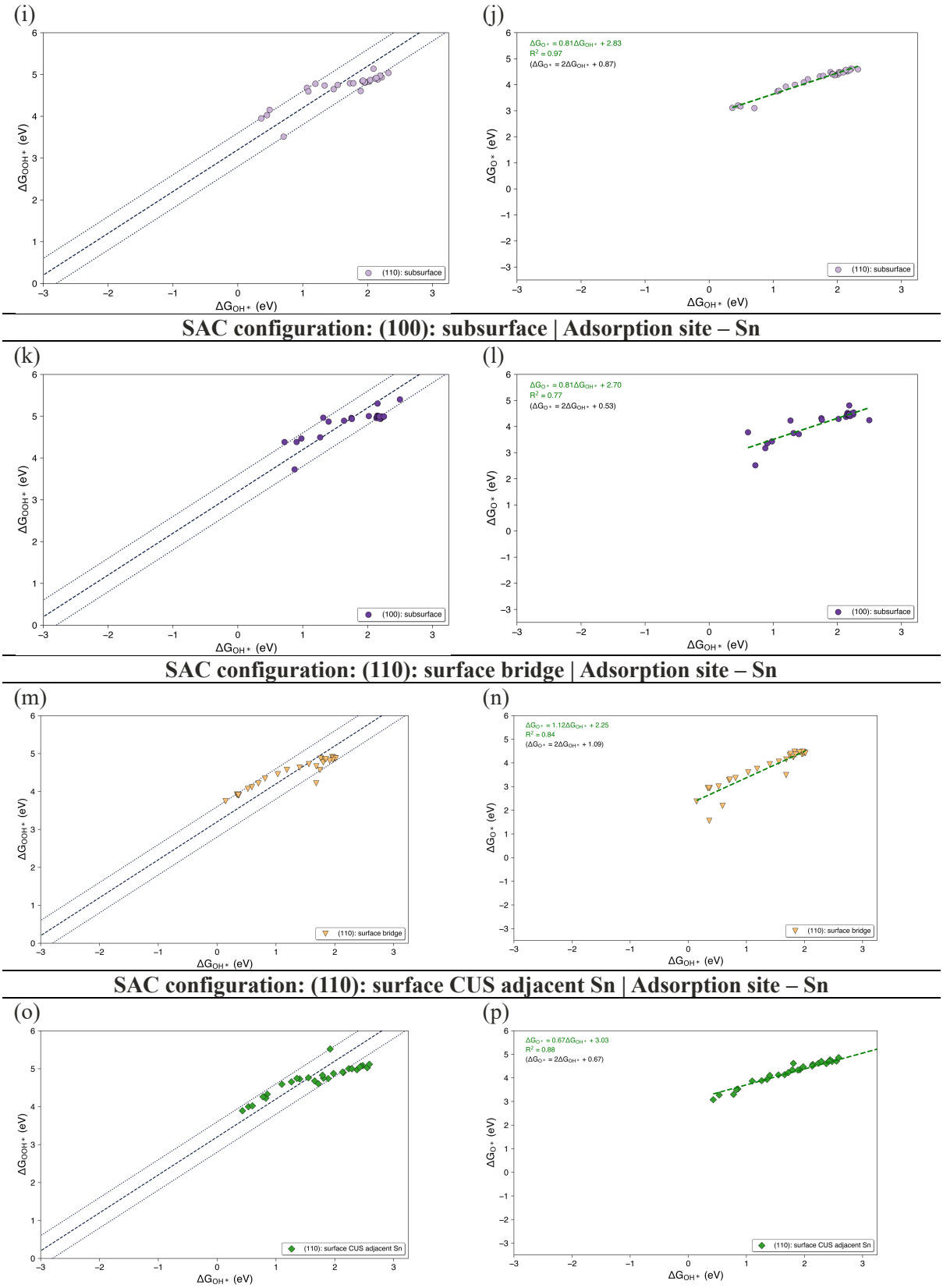


Figure S7. Scaling relations for all the considered SAC configurations. (a–b) SnO_2(110): surface CUS, (c–d) SnO_2(100): surface, (e–f) SnO_2(110): adatom, (g–h) SnO_2(100): adatom, (i–j) SnO_2(110): subsurface, (k–l) SnO_2(100): subsurface, (m–n) SnO_2(110): surface bridge, and (o–p) SnO_2(110):surface CUS adjacent Sn. Each pair shows scaling relations of ΔG_{OOH*} vs. ΔG_{OH*} and ΔG_{O*} vs. ΔG_{OH*}, respectively.

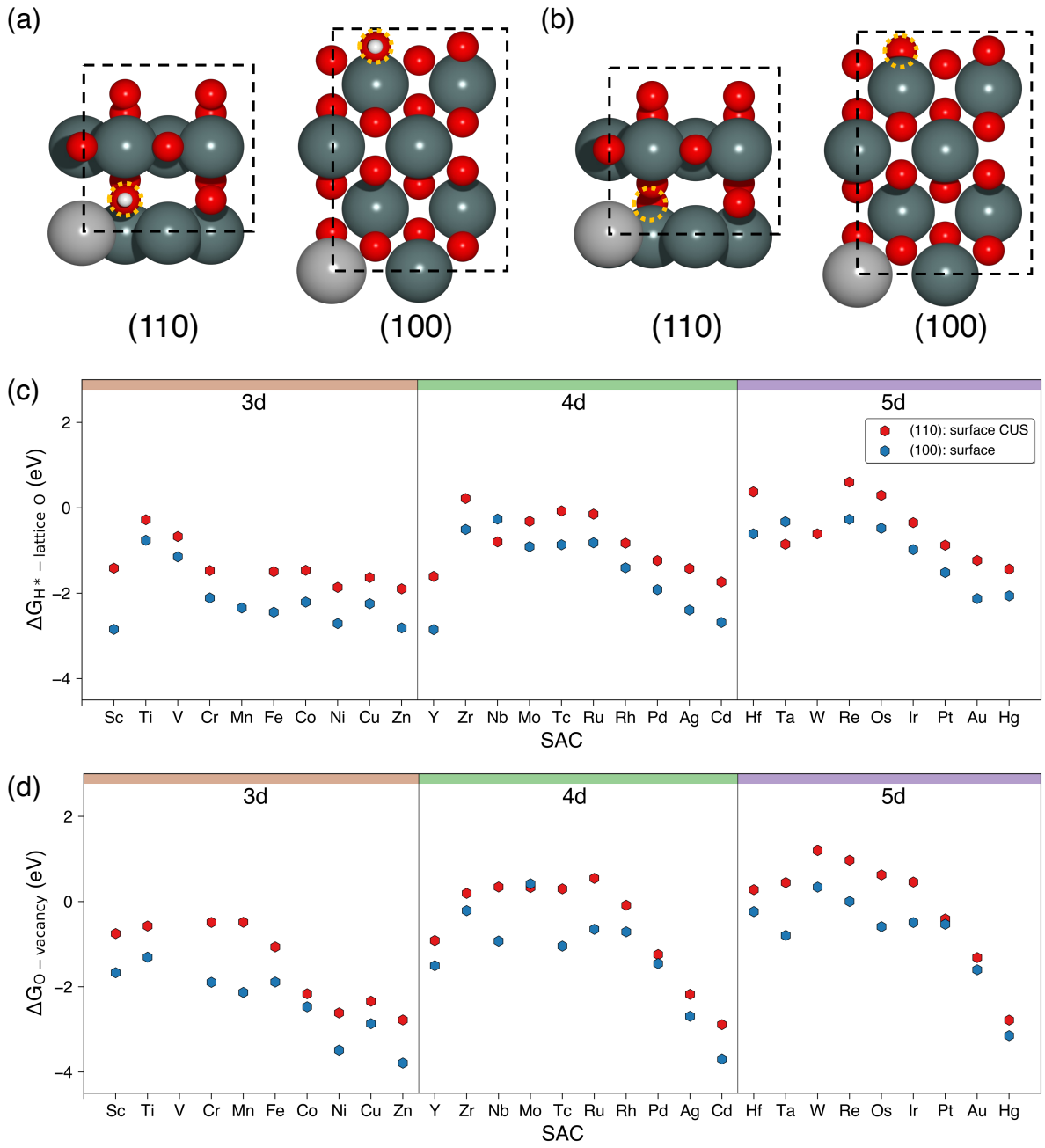


Figure S8. Adsorption energy trend of H* on lattice O and O-vacancy formation on SnO_2(110): surface CUS, and SnO_2(100): surface. Atomic figures of (a) H* adsorption (b) O-vacancies on SnO_2(110): surface CUS, and SnO_2(100): surface**.** Orange circle represents the location of oxygen atom which H* is adsorbed and is removed to form O-vacancies. Free energies of adsorption of (c) H* on lattice-O which is adjacent to surface doped SACs and (d) free energies for O-vacancy creation as function of TM SACs. Note that the oxygen atom which is removed to form an O-vacancy is the same oxygen on which H* is adsorbed. Color code: dark gray – Sn, red – oxygen, light gray - Ag and white – H.

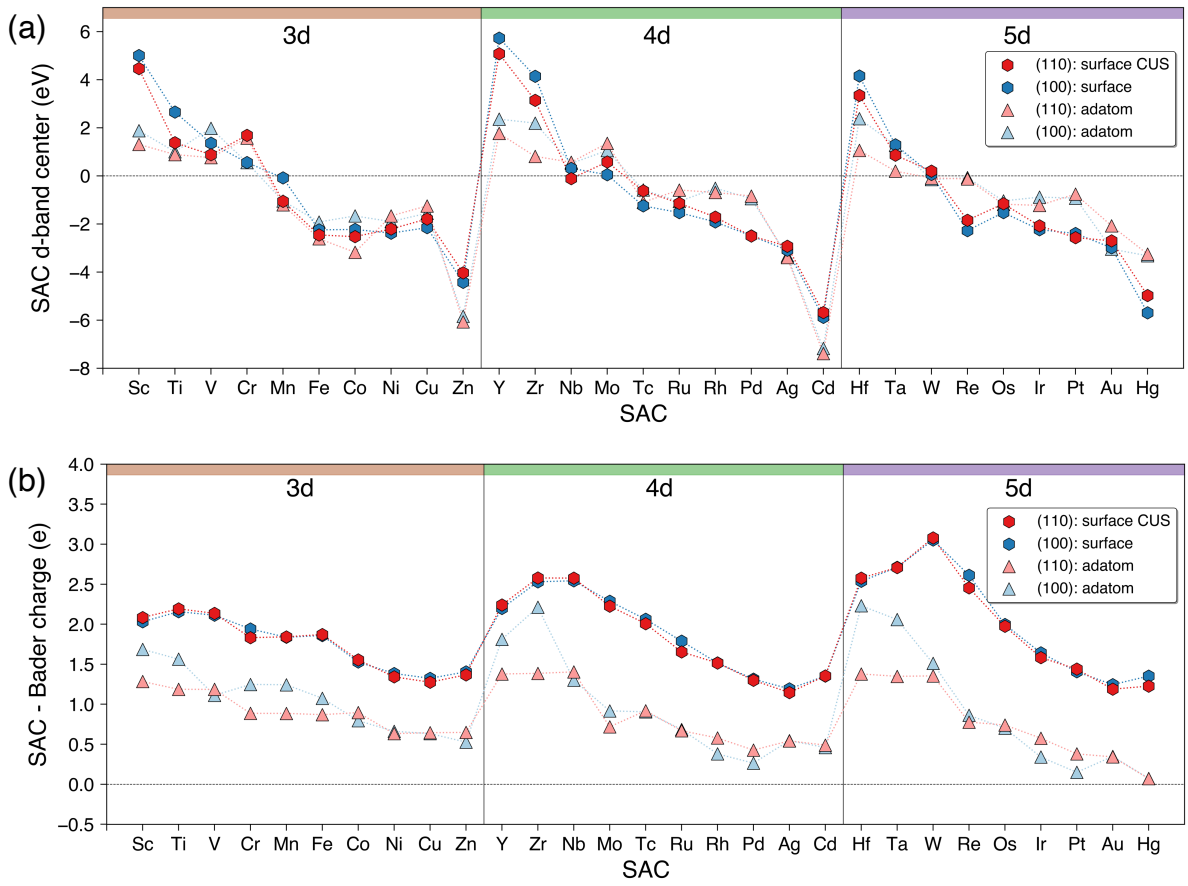


Figure S9. TM–SAC d-band center and SAC Bader charges trends on SnO_2(110): surface CUS, SnO_2(100): surface, SnO_2(110): adatom and SnO_2(100): adatom configurations. (a) TM–SAC d-band center and (b) Bader charge variations as a function of TM–SACs. Bader charges and TM–SAC d-band centers were calculated in the absence of any adsorbates.

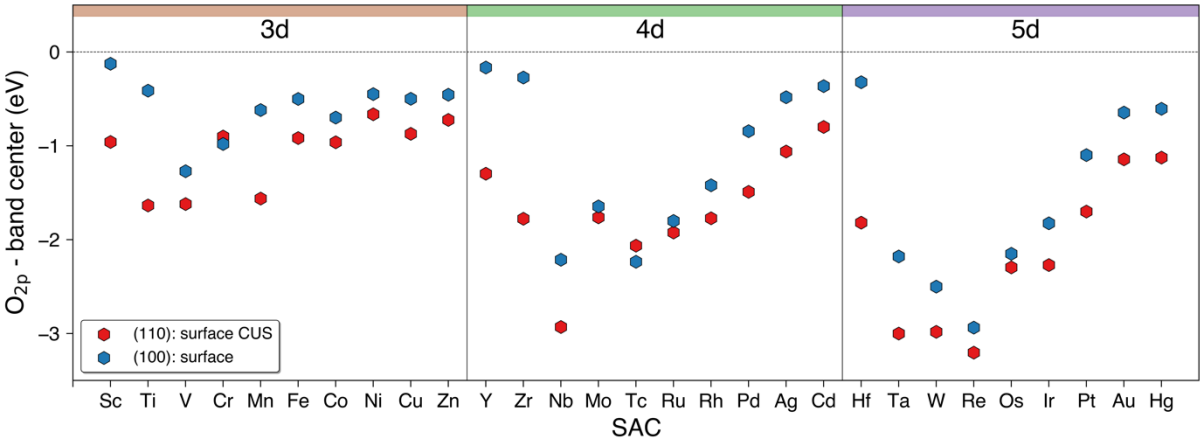


Figure S10. O_{2p} band center trends on SnO_2(110): surface CUS, and SnO_2(100): surface. O_{2p} band centers were calculated for the oxygen atom which is adjacent to the surface SAC atom in the absence of any adsorbates. Note that this oxygen is the same as oxygen considered in **Figure S8**.

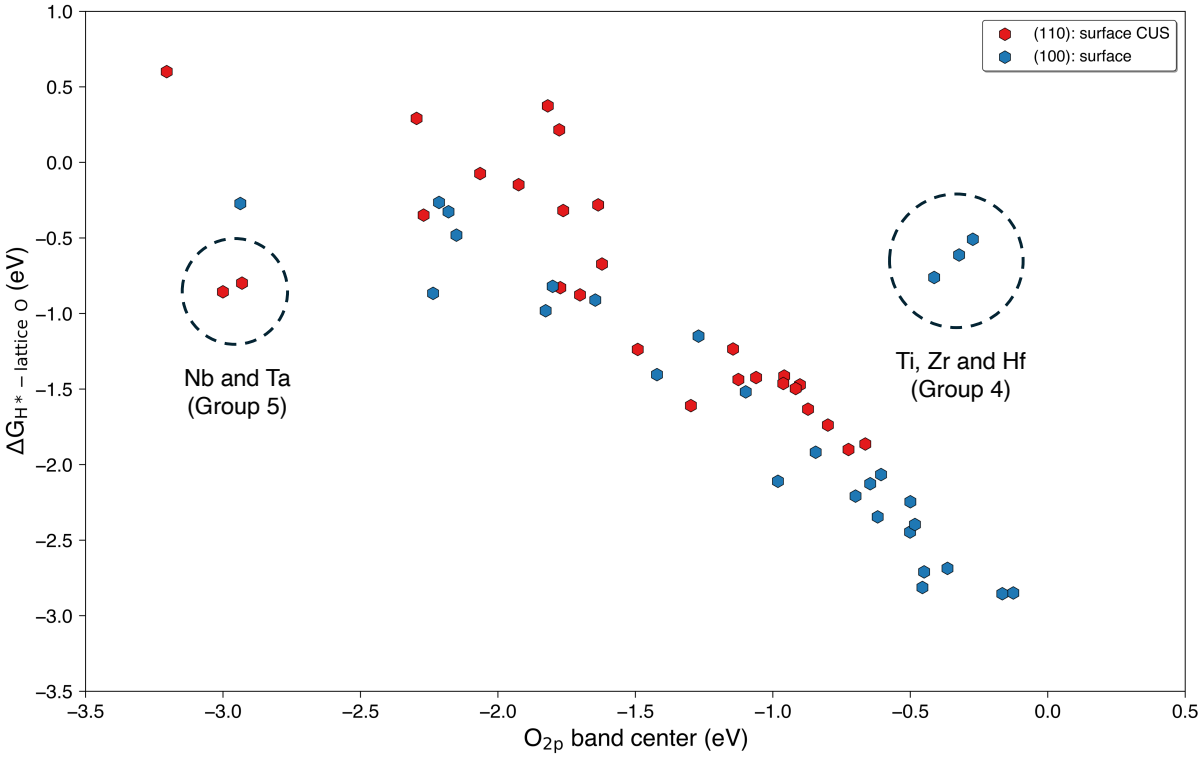


Figure S11. Correlation between H* free energies on lattice O and O_{2p} band centers of SnO_2(110): surface CUS, and SnO_2(100): surface. O_{2p} band centers were calculated for the oxygen which is adjacent to surface doped SAC atom in the absence of any adsorbates, ie. clean surface. Note that this oxygen is the same as oxygen considered in **Figure S8**. Ti, Zr, Hf from group 4 and Nb, Ta for group 5 tend to deviate from the major trend as marked in the figure.

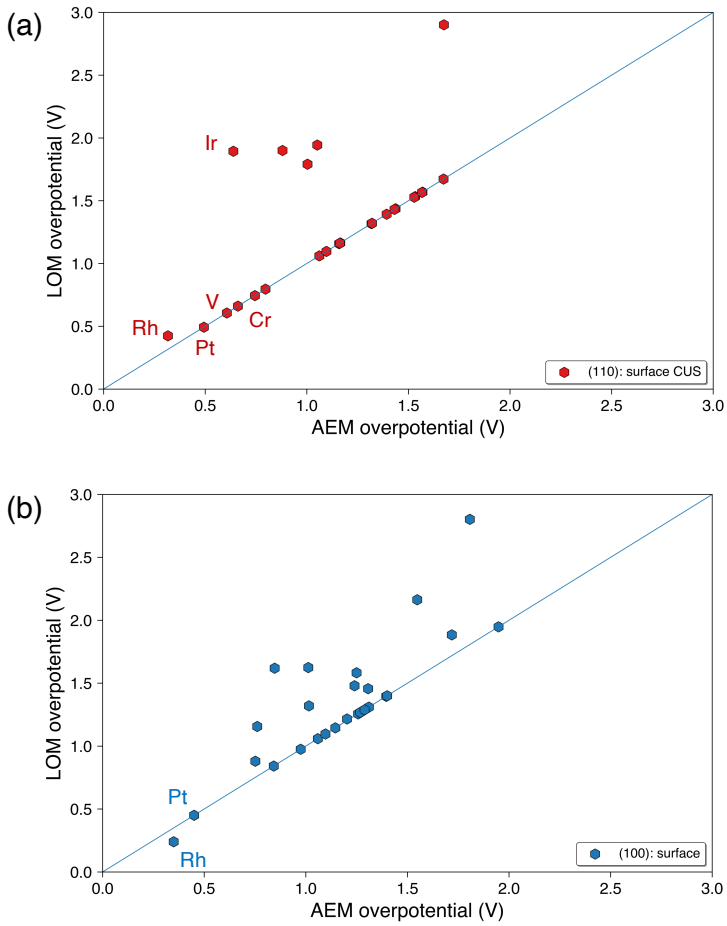


Figure S12. Comparison of AEM (adsorbate evolving mechanism) and LOM (lattice oxygen mechanism) OER overpotentials. LOM overpotential vs AEM overpotential for (a) SnO_2(110): surface CUS and (b) SnO_2(100): surface.

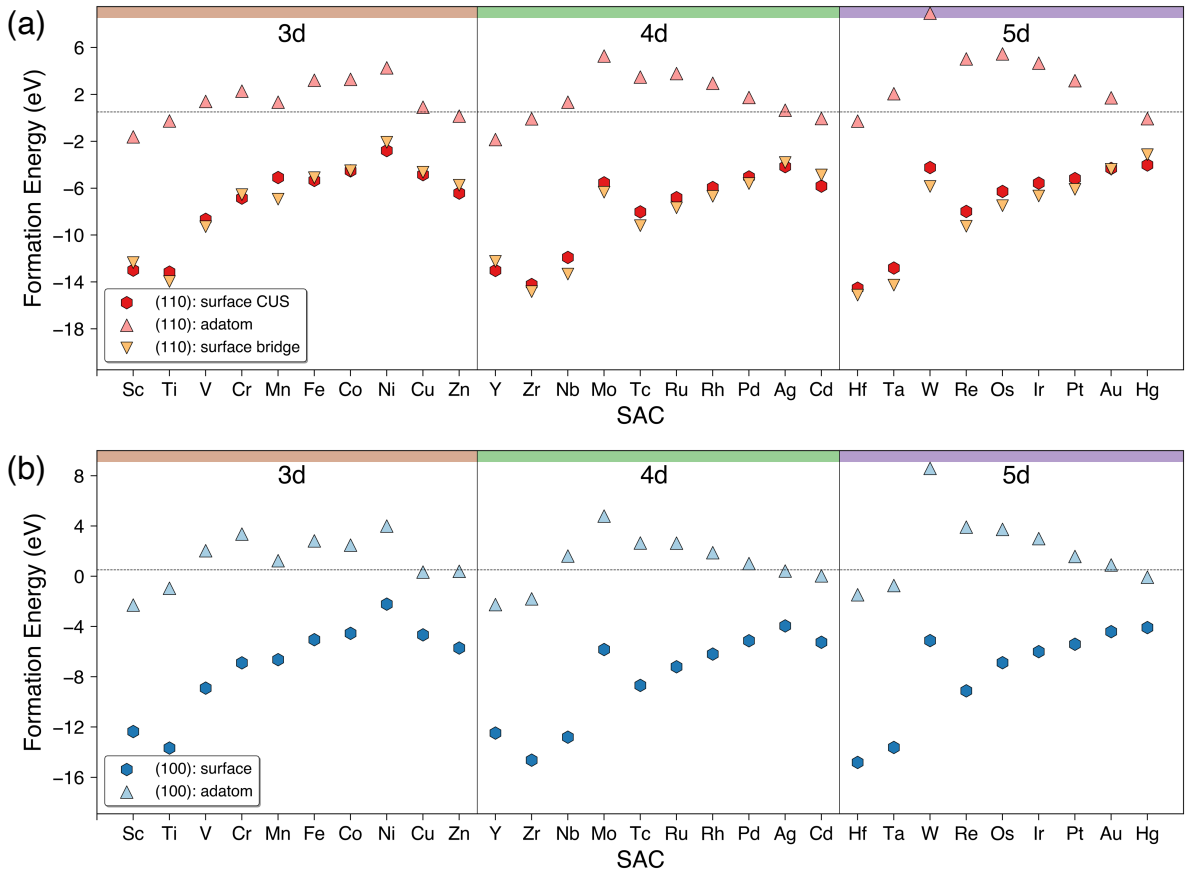


Figure S13. Formation energies of TM–SACs on SnO_2(110) and SnO_2(100) based on metal references. Formation energies of (a) SnO_2(110): surface CUS, SnO_2(110): adatom, SnO_2(110): surface bridge and configurations (b) SnO_2(100): surface and SnO_2(100): adatom configurations. The dashed line at 0.5 eV in formation energy figures denotes the stability threshold under which all SACs are considered to be potentially stable. Formation energies for surface SACs configurations were calculated considering a surface Sn vacancy site on SnO_2(100) and SnO_2(110) as the initial state according to the **reaction 11** while formation energies of surface adatoms were calculated using **reaction 12** in the main manuscript. Reference for the TM–SAC is bulk metallic materials tabulated in **Table S10**.

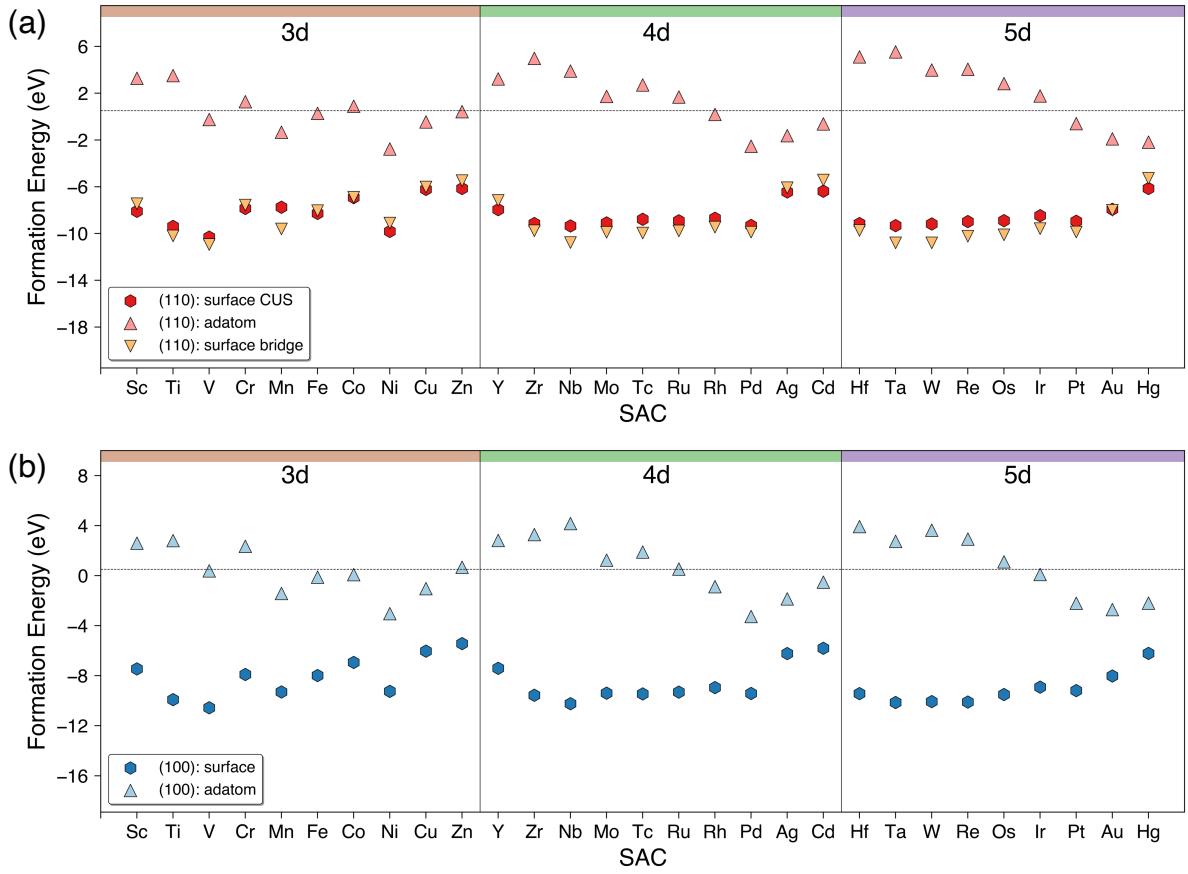


Figure S14. Formation energies of TM–SACs on SnO_2(110) and SnO_2(100) based on metal-oxide references. Formation energies of (a) SnO_2(110): surface CUS, SnO_2(110): adatom, SnO_2(110): surface bridge and, (b) SnO_2(100): surface and SnO_2(100): adatom configurations. The dashed line at 0.5 eV in formation energy figures denotes the stability threshold under which all SACs are considered to be potentially stable. Formation energies for surface SACs configurations were calculated considering a surface Sn vacancy site on SnO_2(100) and SnO_2(110) as the initial state according to the **reaction 1** while formation energies of surface adatoms were calculated using **reaction 2**. Reference for the TM–SAC is bulk oxide materials tabulated in **Table S12**. Reference for the oxygen was taken as $H_2O_{(g)} - H_{2(g)}$.

$$MO_{x\,(bulk)} + Sn_{N-1}O_{2N\,(surface)} \xrightarrow{\Delta E_f} M_{(surface\text{-}doped)}Sn_{N-1}O_{2N\,(surface)} + O_x \qquad (1)$$

$$MO_{x\,(bulk)} + Sn_{N}O_{2N\,(surface)} \xrightarrow{\Delta E_f} M_{(surface\text{-}adatom)}Sn_{N}O_{2N\,(surface)} + O_x \qquad (2)$$

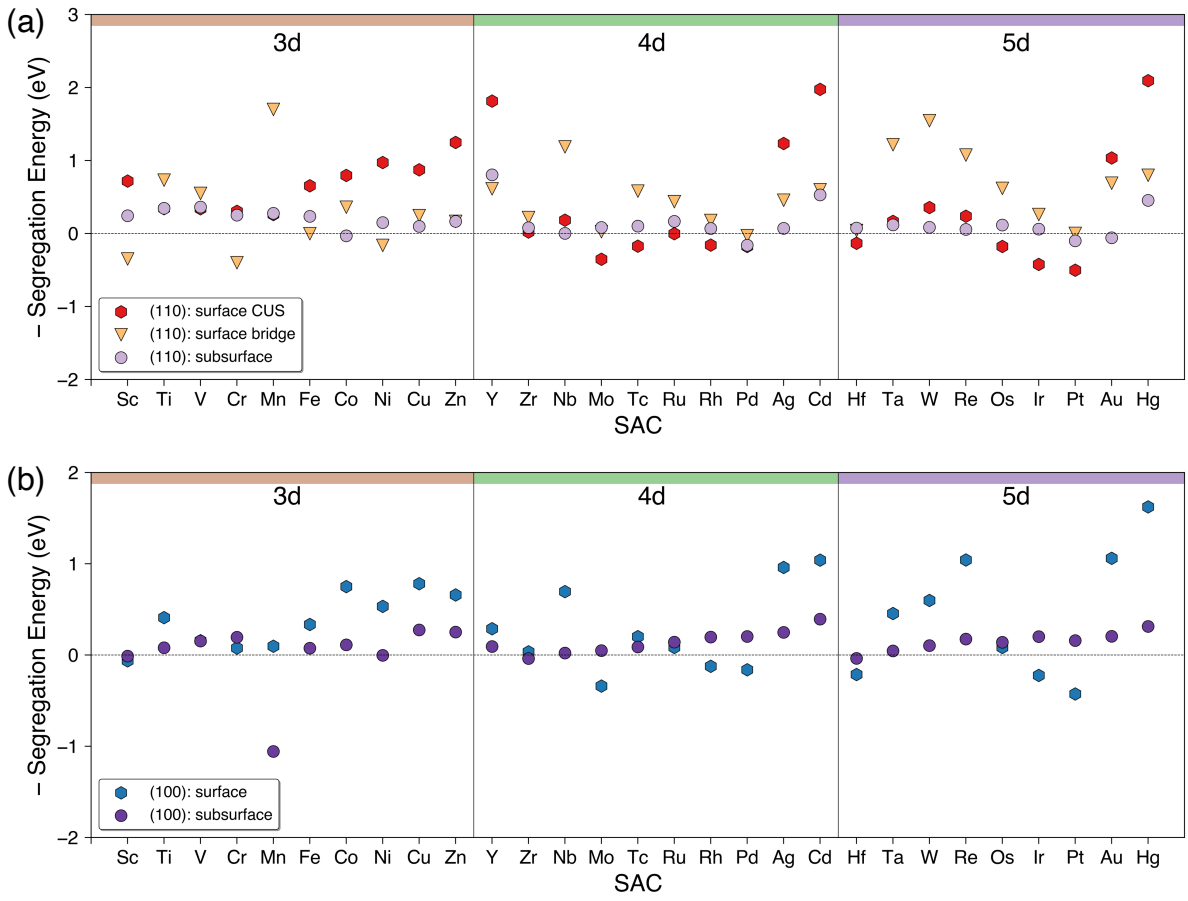


Figure S15. Segregation energies of TM–SACs on SnO_2(110) and SnO_2(100). Negative segregation energies of (a) SnO_2(110): surface CUS, SnO_2(110): surface bridge and SnO_2(110): subsurface (b) SnO_2(100): surface and SnO_2(100): subsurface SACs. Negative segregation energy indicates the favorability for the migration of TM–SACs which are on the surface (or subsurface) to bulk. Positive values represent that TM–SACs are stable on the surface (or subsurface).

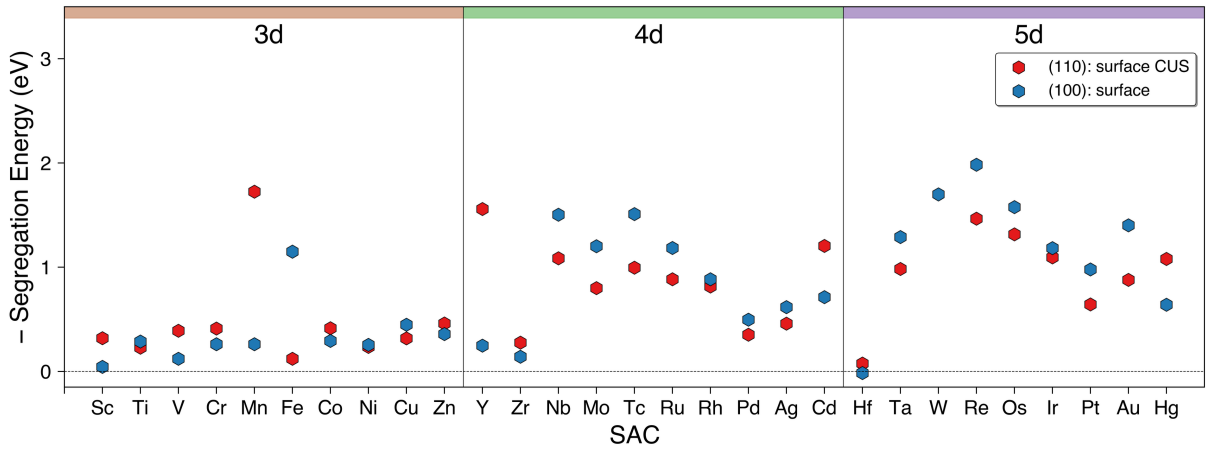


Figure S16. Adsorbate (OH*) induced segregation energies of TM–SACs on SnO_2(110) and SnO_2(100). Negative segregation energy indicates the favorability for the migration of TM–SACs which are on the surface to bulk in the presence of OH*. Positive values represent that SACs are stable on the surface in the presence of OH*.

Table S1. Adsorption free energies of OER intermediates ie. O*, OH* and OOH* (eV), universal scaling gradient ie. $\Delta G_{OOH^*} - \Delta G_{OH^*}$ (eV), OER activity descriptor ie. $\Delta G_{O^*} - \Delta G_{OH^*}$ (eV) and 4e - OER overpotentials (V). Data for all the configurations considered in the current study are included except for 110: bulk and 100: bulk configurations.

Configuration – 110: surface CUS (ads. site - TM)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	4.78	2.38	4.95	2.57	2.39	1.16
Ti	4.43	2.05	4.89	2.85	2.39	1.16
V	3.24	1.84	4.83	2.99	1.40	0.61
Cr	3.35	1.89	4.69	2.80	1.46	0.66
Mn	2.58	0.47	4.68	4.21	2.11	0.88
Fe	4.67	2.55	5.02	2.48	2.12	1.32
Co	4.73	2.39	5.07	2.68	2.34	1.16
Ni	4.85	2.76	5.18	2.42	2.09	1.53
Cu	4.63	2.62	5.18	2.56	2.01	1.39
Zn	5.04	2.80	5.19	2.39	2.24	1.57
Y	4.78	2.23	4.92	2.69	2.55	1.32
Zr	4.43	1.67	5.00	3.32	2.76	1.53
Nb	2.19	0.22	3.79	3.57	1.97	0.74
Mo	1.58	0.43	3.81	3.38	1.15	1.00
Tc	0.71	0.54	3.62	3.08	0.17	1.67
Ru	1.60	0.89	3.88	2.99	0.71	1.05
Rh	2.44	0.89	3.96	3.07	1.55	0.32
Pd	3.44	1.42	4.35	2.94	2.03	0.80
Ag	5.05	2.67	5.18	2.51	2.38	1.44
Cd	5.25	2.80	5.08	2.28	2.45	1.57
Hf	4.33	1.67	4.72	3.05	2.66	1.43
Ta	2.42	0.13	3.75	3.62	2.29	1.06
W	1.31	-0.27	3.46	3.72	1.58	0.91
Re	0.24	-0.02	3.31	3.33	0.26	1.84
Os	0.31	0.08	3.21	3.12	0.23	1.67
Ir	1.45	0.15	3.32	3.16	1.29	0.64
Pt	2.49	0.77	3.79	3.02	1.72	0.49
Au	4.15	1.82	5.18	3.36	2.33	1.10
Hg	5.25	2.90	5.16	2.26	2.34	1.67

Configuration – 100: surface (ads. site - TM)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	4.05	2.08	5.02	2.95	1.97	0.85
Ti	4.48	2.29	4.99	2.70	2.19	1.06
V	3.46	2.20	4.26	2.05	1.25	0.97
Cr	3.90	1.98	4.80	2.82	1.92	0.75
Mn	4.37	1.99	4.77	2.77	2.38	1.15
Fe	4.18	2.43	5.35	2.91	1.75	1.20
Co	4.33	2.63	5.35	2.72	1.70	1.40
Ni	4.77	2.47	5.25	2.78	2.30	1.24
Cu	4.29	2.50	5.17	2.67	1.79	1.27
Zn	4.39	2.48	5.13	2.65	1.91	1.25
Y	4.41	2.24	5.00	2.75	2.17	1.01
Zr	4.65	2.11	4.87	2.76	2.54	1.31
Nb	2.95	0.46	3.69	3.22	2.49	1.26
Mo	0.89	0.21	3.84	3.63	0.68	1.72
Tc	0.66	0.54	3.44	2.90	0.12	1.55
Ru	1.55	0.94	3.79	2.86	0.61	1.02
Rh	2.60	1.13	4.18	3.05	1.47	0.35
Pd	3.57	1.50	-	-	2.07	-
Ag	4.68	2.50	5.14	2.64	2.18	1.27
Cd	4.68	2.54	5.13	2.60	2.14	1.31
Hf	4.62	1.99	4.79	2.81	2.63	1.40
Ta	2.87	0.35	3.67	3.31	2.52	1.29
W	1.11	-0.18	3.55	3.73	1.29	1.21
Re	0.49	0.27	3.75	3.47	0.21	2.03
Os	0.41	0.26	3.44	3.18	0.14	1.81
Ir	1.55	0.48	3.54	3.06	1.07	0.76
Pt	2.43	0.75	3.59	2.84	1.68	0.45
Au	3.96	1.63	4.73	3.09	2.33	1.10
Hg	5.24	3.18	5.21	2.03	2.06	1.95

Configuration – 110: adatom (ads. site - TM)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	-0.81	-2.12	-	-	1.30	-
Ti	-2.00	-2.15	-	-	0.15	-
V	0.32	-0.14	2.60	2.74	0.46	1.09
Cr	1.35	-0.80	2.62	3.42	2.15	1.07
Mn	1.48	-0.69	2.82	3.51	2.17	0.94
Fe	1.17	-0.52	2.67	3.19	1.68	1.02
Co	0.63	-0.88	2.50	3.38	1.50	1.19
Ni	1.86	-0.45	3.03	3.48	2.30	1.07
Cu	2.37	0.48	3.36	2.87	1.88	0.65
Zn	1.98	-0.49	3.08	3.57	2.47	1.24
Y	-0.32	-2.34	1.40	3.74	2.01	2.29
Zr	-2.24	-2.38	-	-	0.14	-
Nb	-1.79	-1.37	-	-	-0.43	-
Mo	-0.70	-0.90	2.50	3.41	0.20	1.97
Tc	-1.62	-1.06	-	-	-0.57	-
Ru	-0.56	-0.59	2.82	3.41	0.03	2.15
Rh	0.62	0.06	2.96	2.90	0.56	1.11
Pd	2.13	0.64	3.61	2.98	1.50	0.27
Ag	3.41	1.08	4.03	2.96	2.33	1.10
Cd	2.74	0.22	3.73	3.51	2.53	1.30
Hf	-1.65	-2.24	-	-	0.59	-
Ta	-2.73	-2.50	-	-	-0.23	-
W	-0.61	-	-	-	-	-
Re	-2.61	-1.59	-	-	-1.02	-
Os	-1.64	-1.44	-	-	-0.20	-
Ir	-0.53	-0.64	-	-	0.11	-
Pt	0.90	-0.43	2.62	3.05	1.33	1.07
Au	2.52	0.01	3.18	3.17	2.51	1.28
Hg	3.96	1.26	4.70	3.44	2.70	1.47

Configuration - 100: adatom (ads. site - TM)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	0.43	-0.96	1.95	2.92	1.39	1.74
Ti	-0.66	-2.60	1.09	3.69	1.94	2.60
V	0.05	-0.57	2.86	3.43	0.61	1.59
Cr	-0.09	-1.32	2.06	3.38	1.23	1.63
Mn	2.17	0.02	3.41	3.39	2.15	0.92
Fe	2.54	0.09	3.61	3.52	2.45	1.22
Co	2.54	0.40	3.77	3.37	2.14	0.91
Ni	2.98	0.42	3.80	3.39	2.56	1.33
Cu	2.92	0.96	4.15	3.19	1.95	0.72
Zn	2.09	-0.34	3.39	3.73	2.43	1.20
Y	0.47	-1.71	1.69	3.41	2.19	2.00
Zr	-0.07	-2.19	-	-	2.11	-
Nb	-1.89	-3.23	-	-	1.34	-
Mo	0.17	0.03	3.36	3.34	0.14	1.97
Tc	-1.10	-0.77	-	-	-0.33	-
Ru	0.06	-0.24	2.67	2.91	0.30	1.38
Rh	1.15	0.11	3.19	3.08	1.04	0.81
Pd	2.92	1.00	4.04	3.04	1.92	0.69
Ag	3.59	1.44	4.43	2.99	2.15	0.92
Cd	3.05	0.64	4.08	3.44	2.41	1.18
Hf	-0.08	-2.76	-	-	2.68	-
Ta	0.02	-1.59	-	-	1.61	-
W	-1.36	-2.37	-	-	1.01	-
Re	-2.00	-1.52	-	-	-0.48	-
Os	-0.66	-0.62	2.14	2.76	-0.04	1.57
Ir	0.45	-0.40	2.72	3.12	0.85	1.04
Pt	2.28	0.54	3.74	3.20	1.74	0.51
Au	2.85	1.03	5.25	4.22	1.82	1.17
Hg	3.74	1.56	5.20	3.64	2.17	0.94

Configuration – 110: subsurface (ads. site - Sn)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	4.52	2.16	4.88	2.73	2.36	1.13
Ti	4.48	2.02	4.83	2.81	2.46	1.23
V	4.39	2.01	4.83	2.83	2.39	1.16
Cr	4.46	2.04	4.87	2.83	2.42	1.19
Mn	3.10	0.70	3.51	2.81	2.40	1.17
Fe	4.62	2.22	4.93	2.72	2.40	1.17
Co	4.48	1.89	4.61	2.71	2.59	1.36
Ni	4.60	2.32	5.04	2.72	2.27	1.09
Cu	4.52	2.12	4.90	2.79	2.41	1.18
Zn	4.56	2.19	4.97	2.78	2.37	1.14
Y	4.48	2.09	5.14	3.05	2.39	1.16
Zr	4.39	1.95	4.81	2.87	2.44	1.21
Nb	3.21	0.45	4.03	3.58	2.76	1.53
Mo	3.93	1.20	4.78	3.58	2.73	1.50
Tc	3.75	1.07	4.68	3.62	2.68	1.45
Ru	4.21	1.54	4.75	3.21	2.67	1.44
Rh	4.32	1.73	4.79	3.06	2.59	1.36
Pd	4.37	1.96	4.81	2.85	2.41	1.18
Ag	4.41	1.92	4.85	2.93	2.49	1.26
Cd	4.57	2.13	4.92	2.79	2.44	1.21
Hf	4.37	1.96	4.82	2.86	2.41	1.18
Ta	3.11	0.36	3.95	3.59	2.75	1.52
W	-	-	3.78	-	-	-
Re	3.17	0.49	4.16	3.67	2.68	1.45
Os	3.77	1.09	4.60	3.51	2.68	1.45
Ir	4.00	1.34	4.74	3.40	2.66	1.43
Pt	4.34	1.78	4.79	3.01	2.56	1.33
Au	4.09	1.48	4.65	3.17	2.62	1.39
Hg	4.41	1.93	4.86	2.93	2.48	1.25

Configuration – 100: subsurface (ads. site - Sn)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	4.37	2.14	4.96	2.82	2.24	1.01
Ti	4.45	2.16	4.98	2.82	2.30	1.07
V	4.46	2.15	5.00	2.85	2.31	1.08
Cr	4.45	2.15	5.01	2.87	2.31	1.08
Mn	3.17	0.87	3.73	2.85	2.30	1.07
Fe	4.44	2.17	5.00	2.84	2.28	1.05
Co	4.52	2.16	4.99	2.84	2.37	1.14
Ni	4.25	2.50	5.40	2.91	1.75	1.27
Cu	4.47	2.15	5.31	3.15	2.31	1.08
Zn	4.49	2.22	4.99	2.78	2.28	1.05
Y	4.40	2.20	4.94	2.74	2.20	0.97
Zr	4.49	2.20	4.95	2.76	2.29	1.06
Nb	3.43	0.98	4.47	3.49	2.45	1.22
Mo	3.75	1.32	4.96	3.65	2.44	1.21
Tc	3.71	1.40	4.87	3.47	2.31	1.08
Ru	4.32	1.75	4.96	3.21	2.57	1.34
Rh	4.29	2.02	5.00	2.99	2.28	1.05
Pd	4.46	2.17	5.00	2.83	2.29	1.06
Ag	4.45	2.17	4.98	2.80	2.28	1.05
Cd	4.46	2.25	4.99	2.74	2.22	1.02
Hf	4.81	2.18	4.94	2.76	2.63	1.40
Ta	3.36	0.90	4.38	3.48	2.45	1.22
W	3.78	0.60	-	-	3.18	-
Re	2.52	0.72	4.38	3.66	1.80	0.63
Os	4.23	1.27	4.50	3.23	2.97	1.74
Ir	-	1.64	4.89	3.26	-	-
Pt	4.46	2.18	4.99	2.81	2.28	1.05
Au	4.26	1.76	4.94	3.18	2.50	1.27
Hg	4.54	2.25	4.99	2.74	2.29	1.06

Configuration – 110: surface bridge (ads. site - Sn)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	4.14	1.69	4.66	2.98	2.46	1.23
Ti	4.45	1.99	4.88	2.89	2.46	1.23
V	3.36	0.81	4.34	3.53	2.55	1.32
Cr	3.49	1.68	4.22	2.53	1.80	0.57
Mn	4.25	1.81	4.83	3.02	2.44	1.21
Fe	4.42	2.00	4.88	2.89	2.43	1.20
Co	4.37	1.96	4.91	2.95	2.41	1.18
Ni	4.32	1.75	4.57	2.82	2.57	1.34
Cu	4.39	1.97	4.89	2.91	2.42	1.19
Zn	4.41	2.02	4.88	2.86	2.40	1.17
Y	4.38	1.76	4.87	3.11	2.62	1.39
Zr	4.48	1.97	4.83	2.87	2.51	1.28
Nb	2.93	0.37	3.91	3.54	2.56	1.33
Mo	2.94	0.34	3.92	3.59	2.60	1.37
Tc	2.19	0.59	4.11	3.52	1.60	0.70
Ru	3.28	0.70	4.21	3.51	2.58	1.35
Rh	3.60	1.03	4.46	3.42	2.57	1.34
Pd	4.05	1.56	4.72	3.16	2.49	1.26
Ag	4.25	1.80	4.77	2.96	2.45	1.22
Cd	4.48	1.83	4.85	3.02	2.65	1.42
Hf	4.45	1.91	4.81	2.90	2.54	1.31
Ta	2.94	0.35	3.90	3.55	2.59	1.36
W	-	0.14	3.74	3.60	-	-
Re	1.55	0.36	3.90	3.54	1.19	1.12
Os	3.00	0.52	4.07	3.55	2.48	1.25
Ir	3.30	0.72	-	-	2.58	-
Pt	3.75	1.19	4.57	3.38	2.56	1.33
Au	3.95	1.40	4.63	3.23	2.55	1.32
Hg	4.35	1.85	4.85	3.00	2.50	1.27

Configuration – 110: surface CUS adjacent Sn (ads. site - Sn)						
TM - SAC	**ΔG_{O^*}**	**ΔG_{OH^*}**	**ΔG_{OOH^*}**	**$\Delta G_{OOH^*} - \Delta G_{OH^*}$**	**$\Delta G_{O^*} - \Delta G_{OH^*}$**	**4e - OER overpotential**
Sc	4.62	2.24	5.00	2.76	2.38	1.15
Ti	4.14	1.66	4.68	3.02	2.48	1.25
V	4.11	1.40	4.73	3.33	2.70	1.47
Cr	4.35	1.92	5.52	3.60	2.43	1.20
Mn	4.62	3.35	4.89	1.53	1.26	2.12
Fe	4.57	2.14	4.90	2.76	2.43	1.20
Co	4.23	1.72	4.60	2.88	2.51	1.28
Ni	4.70	2.47	5.08	2.61	2.22	1.24
Cu	4.51	2.13	4.91	2.78	2.37	1.14
Zn	4.61	2.38	4.97	2.60	2.23	1.15
Y	4.77	2.44	5.07	2.63	2.33	1.21
Zr	4.33	1.89	4.74	2.85	2.45	1.22
Nb	3.28	0.53	4.00	3.47	2.75	1.52
Mo	3.53	0.85	4.33	3.48	2.68	1.45
Tc	3.50	0.83	4.22	3.39	2.68	1.45
Ru	3.94	1.36	4.75	3.39	2.58	1.35
Rh	4.13	1.55	4.76	3.21	2.58	1.35
Pd	4.48	1.98	4.88	2.90	2.50	1.27
Ag	4.71	2.42	5.04	2.62	2.29	1.19
Cd	4.71	2.55	5.03	2.47	2.16	1.32
Hf	4.62	1.81	4.75	2.94	2.81	1.58
Ta	3.08	0.43	3.89	3.46	2.65	1.42
W	-	0.60	4.02	3.42	-	-
Re	3.30	0.78	4.26	3.48	2.52	1.29
Os	3.87	1.10	4.59	3.49	2.77	1.54
Ir	3.89	1.26	4.66	3.39	2.62	1.39
Pt	4.34	1.79	4.83	3.04	2.55	1.32
Au	4.70	2.29	5.00	2.71	2.41	1.18
Hg	4.86	2.59	5.12	2.53	2.28	1.36

Table S2. Adsorption free energies of OH* for 110: bulk and 100: bulk configurations. Note that the adsorption site is Sn for both of these configurations.

	ΔG_{OH^*} (eV)	
TM–SAC	**110: bulk**	**100: bulk**
Sc	1.99	2.19
Ti	1.93	2.17
V	1.89	2.17
Cr	2.00	2.17
Mn	1.94	2.16
Fe	2.02	3.25
Co	2.01	2.17
Ni	2.03	2.19
Cu	2.07	2.17
Zn	2.01	2.18
Y	1.98	2.20
Zr	1.93	2.21
Nb	1.12	1.27
Mo	1.58	1.76
Tc	1.71	1.85
Ru	1.78	2.04
Rh	1.87	2.14
Pd	1.95	2.16
Ag	1.89	2.16
Cd	2.03	2.21
Hf	1.88	2.19
Ta	0.95	1.19
W	-	0.92
Re	1.21	1.22
Os	1.57	1.76
Ir	1.67	1.89
Pt	1.91	2.16
Au	1.66	1.98
Hg	1.89	2.20

Table S3. Adsorption free energies of H* on lattice O which is adjacent to the surface TM-SAC and free energy for oxygen vacancy formation for 110: surface CUS and 100: surface configurations.

	110: surface CUS		100: surface	
TM - SAC	$\Delta G_{H^* - \text{lattice O}}$	$\Delta G_{O - \text{vacancy}}$	$\Delta G_{H^* - \text{lattice O}}$	$\Delta G_{O - \text{vacancy}}$
Sc	-1.41	-0.75	-2.85	-1.67
Ti	-0.28	-0.57	-0.76	-1.31
V	-0.67	-	-1.15	-
Cr	-1.47	-0.49	-2.11	-1.90
Mn	-3.13	-0.49	-2.35	-2.13
Fe	-1.50	-1.07	-2.45	-1.89
Co	-1.46	-2.16	-2.21	-2.47
Ni	-1.86	-2.61	-2.71	-3.49
Cu	-1.63	-2.34	-2.25	-2.87
Zn	-1.90	-2.78	-2.81	-3.79
Y	-1.61	-0.91	-2.85	-1.51
Zr	0.22	0.19	-0.51	-0.21
Nb	-0.80	0.34	-0.26	-0.93
Mo	-0.32	0.33	-0.91	0.42
Tc	-0.07	0.30	-0.87	-1.05
Ru	-0.15	0.54	-0.82	-0.65
Rh	-0.83	-0.08	-1.40	-0.71
Pd	-1.24	-1.24	-1.92	-1.45
Ag	-1.42	-2.18	-2.40	-2.69
Cd	-1.74	-2.89	-2.69	-3.69
Hf	0.37	0.28	-0.61	-0.24
Ta	-0.86	0.44	-0.33	-0.79
W	-0.61	1.20	-	0.34
Re	0.60	0.97	-0.27	0.00
Os	0.29	0.63	-0.48	-0.59
Ir	-0.35	0.46	-0.98	-0.49
Pt	-0.88	-0.41	-1.52	-0.53
Au	-1.23	-1.31	-2.13	-1.60
Hg	-1.44	-2.78	-2.07	-3.15

Table S4. O_{2p} band center trends on SnO_2(110): surface CUS, and SnO_2(100): surface. O_{2p} band centers were calculated for the oxygen atom which is adjacent to the surface TM–SAC in the absence of any adsorbates, ie. clean surface.

	O_{2p} band center (eV)	
TM–SAC	**110: surface CUS**	**100: surface**
Sc	-0.96	-0.13
Ti	-1.64	-0.41
V	-1.62	-1.27
Cr	-0.90	-0.98
Mn	-1.56	-0.62
Fe	-0.92	-0.50
Co	-0.96	-0.70
Ni	-0.66	-0.45
Cu	-0.87	-0.50
Zn	-0.72	-0.46
Y	-1.30	-0.17
Zr	-1.78	-0.27
Nb	-2.93	-2.21
Mo	-1.76	-1.65
Tc	-2.06	-2.24
Ru	-1.92	-1.80
Rh	-1.77	-1.42
Pd	-1.49	-0.84
Ag	-1.06	-0.48
Cd	-0.80	-0.36
Hf	-1.82	-0.32
Ta	-3.00	-2.18
W	-2.98	-2.50
Re	-3.20	-2.94
Os	-2.30	-2.15
Ir	-2.27	-1.83
Pt	-1.70	-1.10
Au	-1.14	-0.65
Hg	-1.13	-0.61

Table S5. SAC d-band centers on SnO_2(110): surface CUS, SnO_2(100): surface, SnO_2(110): adatom and SnO_2(100): adatom configurations. TM–SAC d-band centers were calculated in the absence of any adsorbates, ie. clean surface. Note that TM is the adsorption site for all the configurations mentioned in the table.

	SAC d-band center (eV)			
TM–SAC	**110: surface CUS**	**100: surface**	**110: adatom**	**100: adatom**
Sc	4.46	5.00	1.31	1.88
Ti	1.38	2.65	0.88	1.00
V	0.88	1.36	0.76	1.98
Cr	1.68	0.55	1.57	0.55
Mn	-1.06	-0.09	-1.20	-1.05
Fe	-2.46	-2.25	-2.61	-1.92
Co	-2.53	-2.23	-3.18	-1.67
Ni	-2.21	-2.38	-1.67	-1.90
Cu	-1.80	-2.15	-1.25	-1.56
Zn	-4.04	-4.43	-6.07	-5.84
Y	5.08	5.73	1.76	2.36
Zr	3.14	4.14	0.81	2.19
Nb	-0.12	0.31	0.56	0.51
Mo	0.58	0.05	1.36	1.05
Tc	-0.62	-1.25	-1.10	-0.58
Ru	-1.14	-1.53	-0.59	-1.07
Rh	-1.72	-1.92	-0.69	-0.51
Pd	-2.50	-2.50	-0.84	-0.94
Ag	-2.93	-3.09	-3.40	-3.33
Cd	-5.69	-5.88	-7.39	-7.18
Hf	3.35	4.15	1.06	2.38
Ta	0.86	1.29	0.20	1.27
W	0.20	0.06	-0.09	-0.16
Re	-1.85	-2.28	-0.13	-0.07
Os	-1.16	-1.53	-1.18	-1.04
Ir	-2.08	-2.24	-1.23	-0.89
Pt	-2.57	-2.39	-0.76	-0.93
Au	-2.70	-2.99	-2.08	-3.05
Hg	-4.98	-5.69	-3.25	-3.32

Table S6. TM–SAC Bader charges on SnO_2(110): surface CUS, SnO_2(100): surface, SnO_2(110): adatom and SnO_2(100): adatom configurations. Bader charges were calculated in the absence of any adsorbates, ie. clean surface. Note that TM is the adsorption site for all the configurations mentioned in the table.

	SAC – Bader charge (e)			
TM - SAC	**110: surface CUS**	**100: surface**	**110: adatom**	**100: adatom**
Sc	2.08	2.03	1.28	1.69
Ti	2.19	2.16	1.19	1.56
V	2.13	2.11	1.19	1.11
Cr	1.83	1.94	0.89	1.25
Mn	1.84	1.84	0.89	1.24
Fe	1.87	1.86	0.87	1.07
Co	1.55	1.53	0.90	0.79
Ni	1.34	1.38	0.63	0.66
Cu	1.27	1.32	0.64	0.63
Zn	1.37	1.40	0.65	0.53
Y	2.24	2.20	1.38	1.81
Zr	2.58	2.53	1.39	2.21
Nb	2.58	2.54	1.40	1.30
Mo	2.23	2.29	0.72	0.92
Tc	2.01	2.06	0.92	0.90
Ru	1.65	1.79	0.67	0.68
Rh	1.52	1.52	0.58	0.38
Pd	1.30	1.31	0.43	0.26
Ag	1.15	1.19	0.54	0.55
Cd	1.35	1.35	0.49	0.46
Hf	2.58	2.54	1.38	2.23
Ta	2.71	2.71	1.35	2.06
W	3.08	3.05	1.35	1.51
Re	2.45	2.61	0.78	0.86
Os	1.97	2.00	0.74	0.70
Ir	1.58	1.64	0.58	0.34
Pt	1.44	1.41	0.38	0.15
Au	1.19	1.24	0.34	0.35
Hg	1.23	1.35	0.07	0.07

Table S7. Highly active SnO_2 supported SACs for OER. SAC configuration, TM, adsorption site, free energies of OER intermediates (O*, OH* and OOH*) and 4e – OER overpotentials are mentioned in the table.

Configuration	TM–SAC	Adsorption site	ΔG_{O^*} (eV)	ΔG_{OH^*} (eV)	ΔG_{OOH^*} (eV)	4e - OER overpotential (V)
110: adatom	Pd	SAC	2.13	0.64	3.61	0.27
110: surface CUS	Rh	SAC	2.44	0.89	3.96	0.32
100: surface	Rh	SAC	2.60	1.13	4.18	0.35
100: surface	Pt	SAC	2.43	0.75	3.59	0.45
110: surface CUS	Pt	SAC	2.49	0.77	3.79	0.49
100: adatom	Pt	SAC	2.28	0.54	3.74	0.51
110: surface bridge	Cr	Sn	3.49	1.68	4.22	0.57
110: surface CUS	V	SAC	3.24	1.84	4.83	0.61
100: subsurface	Re	Sn	2.52	0.72	4.38	0.63
110: surface CUS	Ir	SAC	1.45	0.15	3.32	0.64
110: adatom	Cu	SAC	2.37	0.48	3.36	0.65
110: surface CUS	Cr	SAC	3.35	1.89	4.69	0.66
100: adatom	Pd	SAC	2.92	1.00	4.04	0.69
110: surface bridge	Tc	Sn	2.19	0.59	4.11	0.70

Table S8. LOM overpotentials on SnO_2(110): surface CUS and SnO_2(100): surface. AEM overpotentials are also mentioned in the table for comparison.

	110: surface CUS		100: surface	
TM–SAC	**LOM overpotential (V)**	**AEM overpotential (V)**	**LOM overpotential (V)**	**AEM overpotential (V)**
Sc	1.16	1.16	1.62	0.85
Ti	1.16	1.16	1.06	1.06
V	0.61	0.61	0.97	0.97
Cr	0.66	0.66	0.88	0.75
Mn	1.90	0.88	1.15	1.15
Fe	1.32	1.32	1.22	1.20
Co	1.16	1.16	1.40	1.40
Ni	1.53	1.53	1.48	1.24
Cu	1.39	1.39	1.27	1.27
Zn	1.57	1.57	1.58	1.25
Y	1.32	1.32	1.62	1.01
Zr	1.53	1.53	1.31	1.31
Nb	0.74	0.74	1.26	1.26
Mo	1.79	1.00	1.88	1.72
Tc	2.90	1.67	2.16	1.55
Ru	1.94	1.05	1.32	1.02
Rh	0.42	0.32	0.24	0.35
Pd	0.80	0.80	0.84	0.84
Ag	1.44	1.44	1.27	1.27
Cd	1.57	1.57	1.46	1.31
Hf	1.43	1.43	1.40	1.40
Ta	1.06	1.06	1.29	1.29
W	1.77	0.91	0.06	1.21
Re	4.05	1.84	2.93	2.03
Os	3.67	1.67	2.80	1.81
Ir	1.89	0.64	1.16	0.76
Pt	0.49	0.49	0.45	0.45
Au	1.10	1.10	1.10	1.10
Hg	1.67	1.67	1.95	1.95

Table S9. Formation energies of TM–SACs on SnO_2(110) and SnO_2(100) based on metal references.

	Formation energy (eV)				
TM–SAC	**110: surface CUS**	**100: surface**	**110: adatom**	**100: adatom**	**110: surface bridge**
Sc	-12.99	-12.35	-1.61	-2.29	-12.35
Ti	-13.16	-13.67	-0.25	-0.96	-13.97
V	-8.66	-8.90	1.41	2.04	-9.29
Cr	-6.84	-6.89	2.29	3.36	-6.55
Mn	-5.08	-6.64	1.34	1.24	-6.94
Fe	-5.34	-5.04	3.22	2.82	-5.10
Co	-4.52	-4.54	3.29	2.49	-4.50
Ni	-2.79	-2.22	4.27	3.99	-2.08
Cu	-4.85	-4.66	0.92	0.34	-4.64
Zn	-6.41	-5.70	0.16	0.40	-5.75
Y	-13.02	-12.47	-1.85	-2.25	-12.24
Zr	-14.22	-14.63	-0.08	-1.79	-14.83
Nb	-11.91	-12.80	1.35	1.61	-13.33
Mo	-5.54	-5.83	5.28	4.79	-6.34
Tc	-8.02	-8.68	3.48	2.65	-9.19
Ru	-6.81	-7.20	3.78	2.64	-7.67
Rh	-5.94	-6.18	2.95	1.88	-6.70
Pd	-5.04	-5.13	1.74	1.01	-5.60
Ag	-4.17	-3.95	0.65	0.43	-3.81
Cd	-5.83	-5.25	-0.06	0.04	-4.87
Hf	-14.53	-14.81	-0.27	-1.47	-15.13
Ta	-12.81	-13.62	2.06	-0.73	-14.28
W	-4.24	-5.12	8.94	8.59	-5.85
Re	-7.99	-9.11	5.04	3.91	-9.24
Os	-6.28	-6.87	5.46	3.73	-7.49
Ir	-5.56	-6.00	4.68	3.00	-6.67
Pt	-5.17	-5.41	3.18	1.57	-6.10
Au	-4.32	-4.40	1.72	0.90	-4.39
Hg	-4.02	-4.08	-0.06	-0.07	-3.15

Table S10. Reference metallic materials for formation energy calculations using metals as reference. TM, selected materials project ID, formula of the unitcell, total number of sites, total energy of the unitcell and energy per atom are tabulated in the table.

TM	Materials Project ID	Formula	Total number of sites	Total energy (eV)	Energy per atom (eV)
Sc	mp-67	Sc_2	2	-11.886	-5.943
Ti	mp-72	Ti_3	3	-22.211	-7.404
V	mp-146	V_2	2	-16.962	-8.481
Cr	mp-90	Cr_2	2	-17.955	-8.977
Mn	mp-35	Mn_{58}	58	-490.742	-8.461
Fe	mp-13	Fe_2	2	-15.541	-7.771
Co	mp-54	Co_2	2	-13.035	-6.517
Ni	mp-23	Ni_4	4	-19.812	-4.953
Cu	mp-30	Cu_4	4	-13.008	-3.252
Zn	mp-79	Zn_2	2	-1.500	-0.750
Y	mp-112	Y_2	2	-12.233	-6.117
Zr	mp-131	Zr_2	2	-16.192	-8.096
Nb	mp-75	Nb_2	2	-19.135	-9.567
Mo	mp-129	Mo_2	2	-20.647	-10.323
Tc	mp-113	Tc_2	2	-19.454	-9.727
Ru	mp-33	Ru_2	2	-17.194	-8.597
Rh	mp-74	Rh_4	4	-26.447	-6.612
Pd	mp-2	Pd_4	4	-18.515	-4.629
Ag	mp-124	Ag_4	4	-8.795	-2.199
Cd	mp-94	Cd_2	2	-0.705	-0.353
Hf	mp-103	Hf_2	2	-19.022	-9.511
Ta	mp-50	Ta_2	2	-22.645	-11.323
W	mp-91	W_2	2	-24.776	-12.388
Re	mp-8	Re_2	2	-23.567	-11.784
Os	mp-49	Os_2	2	-21.178	-10.589
Ir	mp-101	Ir_4	4	-32.826	-8.207
Pt	mp-126	Pt_4	4	-21.898	-5.474
Au	mp-81	Au_4	4	-10.504	-2.626
Hg	mp-975272	Hg_4	4	0.141	0.035

Table S11. Formation energies of TM–SAC on SnO_2(110) and SnO_2(100) based on metal-oxide references.

	Formation energy (eV)				
TM–SAC	**110: surface CUS**	**100: surface**	**110: adatom**	**100: adatom**	**110: surface bridge**
Sc	-8.10	-7.46	3.28	2.61	-7.45
Ti	-9.39	-9.91	3.51	2.81	-10.20
V	-10.31	-10.56	-0.24	0.38	-10.94
Cr	-7.85	-7.90	1.27	2.34	-7.57
Mn	-7.75	-9.30	-1.33	-1.43	-9.61
Fe	-8.28	-7.98	0.28	-0.12	-8.04
Co	-6.92	-6.94	0.89	0.09	-6.90
Ni	-9.82	-9.25	-2.76	-3.04	-9.11
Cu	-6.22	-6.04	-0.46	-1.04	-6.01
Zn	-6.14	-5.43	0.43	0.67	-5.48
Y	-7.96	-7.40	3.22	2.82	-7.17
Zr	-9.14	-9.56	4.99	3.28	-9.76
Nb	-9.35	-10.24	3.90	4.17	-10.78
Mo	-9.10	-9.39	1.73	1.24	-9.89
Tc	-8.78	-9.45	2.72	1.89	-9.96
Ru	-8.92	-9.31	1.68	0.53	-9.78
Rh	-8.70	-8.95	0.19	-0.88	-9.46
Pd	-9.31	-9.41	-2.54	-3.27	-9.88
Ag	-6.44	-6.23	-1.62	-1.85	-6.08
Cd	-6.39	-5.81	-0.62	-0.52	-5.43
Hf	-9.15	-9.42	5.11	3.92	-9.74
Ta	-9.33	-10.14	5.54	2.75	-10.80
W	-9.19	-10.07	4.00	3.64	-10.80
Re	-8.98	-10.10	4.05	2.92	-10.23
Os	-8.90	-9.50	2.83	1.10	-10.12
Ir	-8.48	-8.91	1.76	0.09	-9.58
Pt	-8.95	-9.18	-0.59	-2.20	-9.87
Au	-7.93	-8.02	-1.90	-2.71	-8.00
Hg	-6.15	-6.21	-2.19	-2.19	-5.27

Table S12. Reference oxide materials for formation energy calculation using metal oxides as reference. TM, selected oxide and materials project ID, formula of the unitcell, total number of sites, total energy of the unitcell and energy per metal atom are tabulated in the table.

TM	Oxide & materials Project ID	Formula	Total number of sites	Total energy (eV)	Energy per metal atom (eV)
Sc	Sc_2O_3-mp-216	$Sc_{32}O_{48}$	80	-690.726	-21.585
Ti	TiO_2-mp-2657	Ti_2O_4	6	-50.986	-25.493
V	V_2O_5-mp-25279	V_4O_{10}	14	-98.942	-24.735
Cr	Cr_2O_3-mp-19399	$Cr_{12}O_{18}$	30	-224.475	-18.706
Mn	MnO_2-mp-19395	Mn_4O_8	12	-80.480	-20.120
Fe	Fe_2O_3-mp-19770	$Fe_{12}O_{18}$	30	-186.901	-15.575
Co	CoO-mp-22408	Co_3O_3	6	-33.839	-11.280
Ni	NiO_2-mp-25210	Ni_3O_6	9	-36.743	-12.248
Cu	CuO-mp-1692	Cu_4O_4	8	-36.153	-9.038
Zn	ZnO-mp-2133	Zn_2O_2	4	-16.371	-8.185
Y	Y_2O_3-mp-2652	$Y_{32}O_{48}$	80	-701.766	-21.930
Zr	ZrO_2-mp-2858	Zr_4O_8	12	-109.979	-27.495
Nb	Nb_2O_5-mp-581967	$Nb_{28}O_{70}$	98	-840.865	-30.031
Mo	MoO_2-mp-510536	Mo_4O_8	12	-84.368	-21.092
Tc	TcO_2-mp-33137	Tc_4O_8	12	-93.144	-23.286
Ru	RuO_2-mp-825	Ru_2O_4	6	-41.631	-20.815
Rh	RhO_2-mp-725	Rh_2O_4	6	-36.351	-18.175
Pd	PdO_2-mp-1018886	Pd_2O_4	6	-29.351	-14.676
Ag	AgO-mp-499	Ag_4O_4	8	-28.336	-7.084
Cd	CdO-mp-1132	Cd_4O_4	8	-27.815	-6.954
Hf	HfO_2-mp-352	Hf_4O_8	12	-116.892	-29.223
Ta	Ta_2O_5-mp-10390	Ta_8O_{20}	28	-261.660	-32.708
W	WO_2-mp-19372	W_4O_8	12	-87.071	-21.768
Re	ReO_2-mp-7228	Re_4O_8	12	-100.479	-25.120
Os	OsO_2-mp-996	Os_2O_4	6	-44.577	-22.289
Ir	IrO_2-mp-2723	Ir_2O_4	6	-39.240	-19.620
Pt	PtO_2-mp-1285	Pt_2O_4	6	-32.056	-16.028
Au	Au_2O_3-mp-27253	$Au_{16}O_{24}$	40	-156.110	-9.757
Hg	HgO-mp-124	Hg_4O_4	8	-20.009	-5.002

Table S13. Segregation energies of SnO_2(110): surface CUS, SnO_2(100): surface, SnO_2(110): subsurface, SnO_2(100): subsurface and SnO_2(110): surface bridge configurations. Negative segregation energy indicates the favorability for the migration of TM–SACs which are on the surface (or subsurface) to bulk. Positive values represent that SACs are stable on the surface (or subsurface).

	Negative segregation energy (eV)				
TM - SAC	**110: surface CUS**	**100: surface**	**110: subsurface**	**100: subsurface**	**110: surface bridge**
Sc	0.72	-0.06	0.24	-0.01	-0.35
Ti	0.34	0.41	0.34	0.08	0.73
V	0.34	0.16	0.36	0.15	0.55
Cr	0.30	0.08	0.25	0.19	-0.40
Mn	0.26	0.10	0.28	-1.06	1.70
Fe	0.65	0.33	0.23	0.07	0.00
Co	0.79	0.75	-0.03	0.11	0.36
Ni	0.97	0.53	0.15	0.00	-0.16
Cu	0.87	0.78	0.10	0.27	0.24
Zn	1.25	0.66	0.16	0.25	0.17
Y	1.81	0.29	0.80	0.09	0.61
Zr	0.02	0.03	0.08	-0.04	0.22
Nb	0.18	0.69	0.00	0.02	1.19
Mo	-0.35	-0.34	0.08	0.05	0.02
Tc	-0.17	0.20	0.10	0.09	0.58
Ru	0.00	0.08	0.17	0.14	0.44
Rh	-0.16	-0.12	0.07	0.20	0.18
Pd	-0.18	-0.16	-0.16	0.20	-0.03
Ag	1.23	0.96	0.07	0.25	0.45
Cd	1.97	1.04	0.53	0.39	0.60
Hf	-0.13	-0.21	0.07	-0.04	0.04
Ta	0.17	0.45	0.12	0.04	1.22
W	0.35	0.60	0.08	0.10	1.55
Re	0.24	1.04	0.05	0.17	1.07
Os	-0.18	0.08	0.12	0.14	0.62
Ir	-0.42	-0.22	0.06	0.20	0.26
Pt	-0.50	-0.43	-0.10	0.16	0.00
Au	1.03	1.06	-0.06	0.20	0.69
Hg	2.09	1.62	0.45	0.31	0.80

Table S14. Adsorbate (OH*) induced segregation energies for SnO_2(110): surface CUS and SnO_2(100): surface configurations. Negative segregation energy indicates the favorability for the migration of TM–SACs which are on the surface to bulk. Positive values represent that SACs are stable on the surface.

	Adsorbate (OH*) induced negative segregation energy(eV)	
TM - SAC	**110: surface CUS**	**100: surface**
Sc	0.32	0.04
Ti	0.23	0.29
V	0.39	0.12
Cr	0.41	0.26
Mn	1.72	0.26
Fe	0.12	1.15
Co	0.41	0.29
Ni	0.24	0.26
Cu	0.32	0.45
Zn	0.46	0.36
Y	1.56	0.25
Zr	0.28	0.14
Nb	1.09	1.50
Mo	0.80	1.20
Tc	1.00	1.51
Ru	0.89	1.19
Rh	0.82	0.88
Pd	0.35	0.50
Ag	0.46	0.62
Cd	1.20	0.71
Hf	0.08	-0.01
Ta	0.98	1.29
W	-	1.70
Re	1.47	1.98
Os	1.32	1.58
Ir	1.09	1.18
Pt	0.64	0.98
Au	0.88	1.40
Hg	1.08	0.64

Table S15. Standard reduction potentials (U_M^0), the number of electrons involved in the dissolution of the metal (N_e) and concentration dependent reduction potential ($U_{M(C_M)}$) calculated at 10^{-6} mol/l using the equation 16 in the main manuscript.

TM–SAC	U_M^0	N_e	$U_{M(C_M)}$
Sc	-2.08	3	-2.20
Ti	-1.63	2	-1.81
V	-1.18	2	-1.36
Cr	-0.91	2	-1.09
Mn	-1.19	2	-1.37
Fe	-0.45	2	-0.63
Co	-0.28	2	-0.46
Ni	-0.26	2	-0.44
Cu	0.34	2	0.16
Zn	-0.76	2	-0.94
Y	-2.37	3	-2.49
Zr	-1.45	4	-1.54
Nb	-1.10	3	-1.22
Mo	-0.20	3	-0.32
Tc	1.50	2	1.32
Ru	0.46	2	0.28
Rh	0.60	1	0.25
Pd	0.95	2	0.77
Ag	0.80	1	0.45
Cd	1.50	2	1.32
Hf	-1.55	4	-1.64
Ta	-0.60	3	-0.72
W	0.10	3	-0.02
Re	0.30	2	0.12
Os	0.84	8	0.80
Ir	1.16	3	1.04
Pt	1.18	2	1.00
Au	1.50	3	1.38
Hg	1.50	2	1.32

Table S16. Dissolution potentials (U_{diss}) for SnO_2(110): surface CUS, SnO_2(100): surface, SnO_2(110): adatom, SnO_2(100): adatom and SnO_2(110): surface bridge configurations.

	Dissolution potentials (V_{RHE})				
TM–SAC	**110: surface CUS**	**100: surface**	**110: adatom**	**100: adatom**	**110: surface bridge**
Sc	2.13	1.92	-1.66	-1.43	1.92
Ti	4.77	5.03	-1.68	-1.33	5.18
V	2.97	3.09	-2.06	-2.38	3.29
Cr	2.33	2.36	-2.23	-2.77	2.19
Mn	1.17	1.95	-2.04	-1.99	2.10
Fe	2.04	1.89	-2.24	-2.04	1.92
Co	1.80	1.81	-2.10	-1.70	1.79
Ni	0.96	0.67	-2.57	-2.43	0.60
Cu	2.59	2.49	-0.30	-0.01	2.48
Zn	2.27	1.91	-1.02	-1.14	1.94
Y	1.85	1.67	-1.87	-1.74	1.59
Zr	2.02	2.12	-1.52	-1.09	2.17
Nb	2.75	3.05	-1.67	-1.76	3.23
Mo	1.53	1.63	-2.08	-1.92	1.79
Tc	5.33	5.66	-0.42	0.00	5.92
Ru	3.69	3.88	-1.61	-1.04	4.12
Rh	6.18	6.43	-2.71	-1.63	6.94
Pd	3.29	3.34	-0.10	0.27	3.57
Ag	4.61	4.39	-0.21	0.02	4.25
Cd	4.24	3.95	1.35	1.30	3.76
Hf	1.99	2.06	-1.57	-1.27	2.14
Ta	3.55	3.82	-1.41	-0.47	4.04
W	1.39	1.69	-3.00	-2.88	1.93
Re	4.12	4.68	-2.40	-1.83	4.74
Os	1.58	1.65	0.11	0.33	1.73
Ir	2.90	3.04	-0.52	0.04	3.26
Pt	3.59	3.71	-0.59	0.22	4.05
Au	2.82	2.85	0.81	1.08	2.84
Hg	3.33	3.37	1.35	1.36	2.90

Table S17. Effects of solvation on free energies of adsorption of key OER intermediates based on AEM and LOM mechanisms. Solvation at the metal oxide surfaces was modeled using the implicit solvent method implemented in VASPsol with a dielectric constant of 80 and a Debye screening length of 3 Å.

(a) Free energies of adsorption of O*, OH*, OOH* and H*-lattice O on selected SACs with and without solvation.

Configuration	TM	Adsorption site	ΔG_{OH^*} (eV)	ΔG_{O^*} (eV)	ΔG_{OOH^*} (eV)	$\Delta G_{H^*\text{- lattice O}}$ (eV)
Without Solvation						
110: surface CUS	Ir	SAC	0.15	1.45	3.32	-0.35
110: surface CUS	Rh	SAC	0.89	2.44	3.96	-0.83
110: surface CUS	Pt	SAC	0.77	2.49	3.79	-0.88
100: surface	Rh	SAC	1.13	2.60	4.18	-1.40
100: surface	Pt	SAC	0.75	2.43	3.59	-1.52
With solvation						
110: surface CUS	Ir	SAC	0.25	1.48	3.26	-0.39
110: surface CUS	Rh	SAC	1.03	2.58	3.92	-0.89
110: surface CUS	Pt	SAC	0.75	-	3.67	-0.88
100: surface	Rh	SAC	1.00	2.61	4.15	-1.38
100: surface	Pt	SAC	0.75	2.40	-	-1.50

(b) Solvation energies (eV) of O*, OH*, OOH* and H*-lattice O on selected SACs. Solvation energies were calculated as ΔG_x(with sol.) - ΔG_x(without sol.) where x is the OER intermediate adsorbed on the SAC.

Configuration	TM	Adsorption site	OH*	O*	OOH*	H*- lattice O
110: surface CUS	Ir	SAC	0.09	0.03	-0.05	-0.04
110: surface CUS	Rh	SAC	0.14	0.14	-0.05	-0.07
110: surface CUS	Pt	SAC	-0.01	-	-0.12	-0.01
100: surface	Rh	SAC	-0.12	0.01	-0.03	0.03
100: surface	Pt	SAC	0.00	-0.03	-	0.01

Table S18. Effects of solvation on OER overpotentials based on AEM and LOM mechanisms.

(a) Effect on AEM overpotentials on selected SACs

Configuration	TM	Adsorption site	AEM overpotentials (V)		Difference (eV)
			Without solvation	With solvation	
110: surface CUS	Ir	SAC	0.64	0.55	-0.08
110: surface CUS	Rh	SAC	0.32	0.32	0.00
110: surface CUS	Pt	SAC	0.49	-	-
100: surface	Rh	SAC	0.35	0.37	0.02
100: surface	Pt	SAC	0.45	-	-

(b) Effect on LOM overpotentials on selected SACs

Configuration	TM	Adsorption site	LOM overpotentials (V)		Difference (eV)
			Without solvation	With solvation	
110: surface CUS	Ir	SAC	1.89	1.82	-0.07
110: surface CUS	Rh	SAC	0.42	0.32	-0.11
110: surface CUS	Pt	SAC	0.49	-	-
100: surface	Rh	SAC	0.24	0.37	0.13
100: surface	Pt	SAC	0.45	0.42	-0.03