Supplemental info for "Trends in adsorption of electrocatalytic water splitting intermediates on cubic ABO_3 oxides""

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1 Calculation details

The calculations performed herein used the Quantum Espresso[1] pwscf code for computational of potential energies of both bulk and surface atomic configurations. These calculations use a plane-wave electronic energy cutoff of 400 eV and a density cutoff of 4000 eV. 8x8x8 and 4x4x1 k-point meshes generated according to the Monkhorst-Pack[2] scheme were used for bulk and surface calculations, respectively. Calculations were run non-spin-polarized and with a dipole correction. Slab and adsorbate calculations used a 2x2x3 supercell relative to the 5-atom cubic bulk unit cell, and only the atoms in the topmost layer, along with any adsorbates, were left unconstrained in force optimization. Ionic relaxation to a maximum force of 0.05 eV/Åwas conducted using the LBFGS algorithm as implemented in the Atomic Simulation Environment.[3] As mentioned in the main text, the RBPE[4] functional was used.

Bulk cubic ABO_3 compounds were structurally optimized by fitting isotropic volume perturbations to previously determined lattice constants to find the minimum potential energy lattice. For projected density of states (PDOS) calculations, a non-self-consistent (NSCF) calculation was conducted over a finer (8x8x1) k-point mesh.

2 Free energy corrections

The Gibbs free energy (ΔG) of the adsorbates presented in the main text are determined using corrections enumerated in the Table 1. These include the heat-capacity corrections to the enthalpy, the zero-point energy and the entropy. Corrections to the gas-phase H_2 and liquid phase H_2O are made using the IdealGasThermo class in the ase.thermochemistry module using a temperature of 25^o and pressures of 101325 Pa for H_2 and 3540 Pa for H_2O (the vapor pressure of water, which defines the equilibrium between the gas and liquid phases). These corrections (totaled in the column labeled ΔG_{corr} are added to the electronic energy of the state to represent the total Gibbs free energy of the state, which are then used to calculate the Gibbs free energy of reaction to form the adsorbate from the slab and molecular precursors, *e.g.*

$$\Delta G_{adsorption} = \Delta G_{adsorbate} - \Delta G_{slab} - n\Delta G_{H_2O} - m\Delta G_{H_2}, \quad (1)$$

where n and m are the appropriate coefficients needed to balance the stoichiometry of the chemical reaction for the formation of the adsorbate.

State	$\nu\ (cm^{-1})$	ΔE_{ZPE} (eV)	$\int_0^{300} C_v dT$ (eV)	$T\Delta S$ (eV)	ΔG_{corr} (eV)
$H_2O^{(l)}$	[1584, 3587, 3696]	0.57	0.08	0.66	-0.01
$H_2^{(g)}$	[4274]	0.26	0.09	0.40	-0.05
H*-M	[336, 352, 1210]	0.12	0.02	0.03	0.11
H*-O	[644, 856, 3444]	0.31	0.01	0.01	0.30
O*	[228, 255, 732]	0.08	0.03	0.05	0.06
OH*	[225, 250, 285, 507, 596, 3659]	0.34	0.05	0.08	0.31
OOH*	[158, 222, 241, 289, 304, 331, 1065, 1359, 3466]	0.46	0.08	0.14	0.40

3 Oxygen evolution data

In this supplement, we include the data on oxygen evolution used to generate the figures in the main text. Also included are all data which resulted in failed runs or that can be reconstructed from scaling. Data not explicitly included in the figures are marked with letters in the "warning" column indicating the cause of the failure of the run, which are enumerated below the table.

Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$YRhO_3$	0.80	2.30	3.77	0.26	0.90	None
$BaRuO_3$	0.50	1.96	3.46	0.27	0.42	None
$BaRhO_3$	0.66	2.19	3.52	0.30	0.60	None
$MgRhO_3$	1.05	2.60	3.65	0.32	0.90	a
$ScIrO_3$	0.46	1.95	3.53	0.36	1.54	None
$MgIrO_3$	0.59	2.19	3.72	0.37	1.24	a
$MgBaO_3$	0.57	1.80	3.30	0.39	1.84	a,b
$BaNiO_3$	0.61	2.24	3.74	0.39	0.66	a,b
$KRuO_3$	1.23	2.86	4.16	0.40	0.62	None
$ScRhO_3$	0.83	2.47	3.88	0.41	1.10	a,b
$NaRuO_3$	0.78	2.41	3.92	0.41	0.68	a
$SrPtO_3$	0.99	2.65	3.75	0.43	0.84	a
$AgRuO_3$	0.35	1.85	3.53	0.45	1.22	a,b
$ZrRuO_3$	0.33	1.73	3.43	0.47	1.24	a
$ZrFeO_3$	0.65	2.36	3.77	0.49	1.00	a
$ScAsO_3$	-0.26	1.46	3.21	0.52	1.22	a,b
$LaFeO_3$	0.11	1.66	3.41	0.52	0.14	a
$ZrInO_3$	0.27	1.70	3.46	0.53	0.86	a,b
$ZrCaO_3$	0.70	2.46	3.82	0.53	1.08	a,b
$PbBiO_3$	0.27	1.70	3.46	0.53	0.60	a
$BaIrO_3$	0.84	2.12	3.89	0.54	0.62	None
$InCuO_3$	0.26	1.67	3.45	0.55	1.02	a,b
$BaTeO_3$	-0.27	1.40	3.19	0.56	0.22	b
$NaLaO_3$	1.45	3.00	4.80	0.57	0.90	a,b
$InGaO_3$	0.23	1.62	3.43	0.57	0.60	a,b
$SrNiO_3$	0.64	2.46	3.80	0.59	0.64	a,b
$SrIrO_3$	0.67	1.91	3.73	0.59	0.70	None
$BaPtO_3$	1.12	2.94	3.99	0.60	0.78	None
$AgLaO_3$	0.85	2.69	3.93	0.61	1.38	a,b
$SiNbO_3$	0.18	1.53	3.39	0.62	1.04	a
$PbScO_3$	0.18	1.53	3.38	0.62	0.60	a,b
$SrMnO_3$	0.28	1.60	3.46	0.63	-0.10	a
$SrTeO_3$	-0.25	1.27	3.14	0.64	0.38	b
$BeIrO_3$	1.65	3.08	4.95	0.64	1.56	None

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$CaBO_3$	0.60	2.23	4.13	0.67	0.98	b
$ZrMgO_3$	-0.34	1.56	3.20	0.67	0.56	a,b
$PbBaO_3$	0.89	2.78	3.96	0.67	1.06	a
$CaMnO_3$	0.24	1.53	3.43	0.67	0.00	a
$ZrNaO_3$	0.91	2.82	3.98	0.68	1.30	a
$SrRuO_3$	0.05	1.75	3.00	0.69	0.50	a
$TlIrO_3$	0.94	2.86	4.01	0.69	1.12	a
YBO_3	0.54	2.48	3.13	0.70	0.70	b
$ScRuO_3$	0.65	1.69	3.63	0.71	1.36	a
$PbPbO_3$	0.08	1.36	3.31	0.72	0.72	a,b
$YGeO_3$	-0.31	1.65	3.20	0.73	0.64	b
$PbIrO_3$	-0.26	1.70	3.26	0.74	0.92	a,b
$TlTiO_3$	0.17	1.39	3.37	0.75	0.40	a,b
$HgIrO_3$	1.01	2.99	4.06	0.75	1.36	a
$SrRhO_3$	-0.04	1.93	2.93	0.76	0.68	None
$NaPtO_3$	1.32	3.32	4.43	0.77	1.18	a,b
$PdIrO_3$	1.03	3.03	4.08	0.77	1.64	a
$NaIrO_3$	0.13	1.31	3.33	0.79	0.84	a
$CaBiO_3$	0.73	2.75	3.90	0.79	0.68	a
$ZrReO_3$	-0.01	1.21	3.24	0.80	1.20	a
$LaCoO_3$	0.40	2.43	3.51	0.80	0.30	None
$SrSbO_3$	-0.69	1.26	2.88	0.81	0.18	None
$YNiO_3$	1.27	3.35	3.62	0.84	0.64	None
$HfNiO_3$	1.12	3.19	4.15	0.85	1.26	a
$CaNiO_3$	0.33	2.41	3.66	0.85	0.74	a,b
$CaPtO_3$	-0.09	1.07	3.17	0.87	1.06	a,b
$SrPdO_3$	1.30	3.40	3.82	0.87	0.96	None
$LaNiO_3$	1.39	3.50	4.47	0.88	0.36	None
$ScNiO_3$	1.29	3.39	4.26	0.88	0.94	a
$BaPdO_3$	1.39	3.54	4.15	0.92	0.80	None
$SiTaO_3$	-0.13	0.98	3.13	0.92	0.84	a
$YPdO_3$	-0.09	2.07	2.78	0.92	1.02	b
$KTeO_3$	-0.16	0.98	3.12	0.92	0.38	a,b
$BaGeO_3$	0.44	2.55	2.76	0.93	0.02	b
$PbPtO_3$	0.53	2.70	3.81	0.94	1.06	a,b
$NaNbO_3$	-0.60	0.71	2.90	0.97	-0.32	None
$SbNiO_3$	1.27	3.48	4.28	0.98	0.76	a
$InPdO_3$	-1.20	1.01	2.73	0.98	1.14	a,b
$CdNiO_3$	1.27	3.49	4.28	0.99	1.06	a
$BiNiO_3$	1.27	3.49	4.28	0.99	0.72	a
$PbTiO_3$	1.19	3.42	4.44	1.00	0.06	None

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$SnNiO_3$	1.30	3.53	4.30	1.01	0.80	a
$TlNiO_3$	1.31	3.55	4.31	1.02	1.14	a
$AuNiO_3$	1.32	3.58	4.32	1.03	1.72	a
$AgSbO_3$	0.40	2.67	4.26	1.04	0.76	a
$SrBiO_3$	0.65	2.93	3.56	1.05	0.42	None
$LaRhO_3$	-0.39	1.82	2.64	1.05	0.68	None
$ZrIrO_3$	1.38	3.66	4.39	1.06	1.46	a
$SrBO_3$	0.82	1.99	4.28	1.06	0.96	b
$AlBO_3$	2.30	4.56	5.27	1.07	1.22	None
$BaSbO_3$	-0.99	1.31	2.61	1.08	0.04	None
$ScSrO_3$	1.16	3.48	4.39	1.09	1.30	a
$PbCoO_3$	-0.32	0.65	2.98	1.09	0.74	a,b
$NaTeO_3$	0.18	2.55	3.63	1.13	0.48	b
$ScPdO_3$	1.35	3.72	4.36	1.14	1.54	a
$PbBO_3$	-0.37	0.57	2.94	1.14	1.22	a,b
$YScO_3$	-0.19	1.89	2.55	1.14	0.34	b
$KNbO_3$	-0.65	0.50	2.88	1.15	-0.42	None
$LaPtO_3$	0.45	2.84	3.39	1.16	0.84	None
$ScBO_3$	1.25	2.55	4.95	1.16	0.84	b
$CaTiO_3$	1.44	3.84	4.70	1.17	-0.12	None
$CaSbO_3$	-0.55	1.43	2.52	1.17	0.38	b
$BaAuO_3$	2.01	4.42	4.83	1.18	1.02	None
$BaBiO_3$	0.69	3.10	3.88	1.18	0.28	None
$SrTiO_3$	1.27	3.68	4.49	1.18	-0.24	None
$ZrRhO_3$	-0.45	0.52	2.94	1.19	1.64	a
$ZrMoO_3$	-0.43	0.47	2.89	1.19	0.88	a,b
$MgPdO_3$	1.52	3.95	3.50	1.21	1.10	c
$LaPdO_3$	0.96	3.42	3.78	1.23	0.72	None
$PbRhO_3$	-0.87	1.57	2.46	1.23	0.90	b
$CaCuO_3$	2.03	4.51	5.01	1.25	0.96	None
$LiNbO_3$	-0.77	0.27	2.76	1.26	-0.06	b
$LiVO_3$	-0.36	2.13	4.22	1.26	0.18	b
$SrAuO_3$	1.87	4.37	4.73	1.27	1.12	None
$LaGeO_3$	-0.81	0.20	2.71	1.27	0.28	b
$NaVO_3$	-0.11	2.39	4.51	1.27	0.10	b
$PbNiO_3$	1.13	3.63	4.25	1.27	0.88	a
$PbAlO_3$	1.53	4.04	4.61	1.28	0.52	a
$AlTiO_3$	-0.34	0.42	2.95	1.29	0.54	a
$AgTeO_3$	-0.53	-0.12	2.40	1.29	1.02	a,b
$NaTiO_3$	2.47	4.99	5.14	1.29	0.18	None
$KHgO_3$	2.30	4.83	4.99	1.30	1.44	a

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$KOsO_3$	-0.15	0.49	3.02	1.30	0.50	None
$BaCuO_3$	2.06	4.60	4.99	1.30	0.82	None
$ScCuO_3$	1.95	4.47	4.77	1.30	1.18	a
$KTiO_3$	2.30	4.83	4.97	1.30	0.16	None
$KTaO_3$	-1.15	0.05	2.38	1.31	-0.64	None
$LiSiO_3$	2.16	4.70	5.11	1.31	0.54	None
$AgNbO_3$	-0.59	0.39	2.93	1.31	0.20	None
$LaCuO_3$	2.05	4.59	4.76	1.31	0.54	None
$BaBO_3$	0.86	1.77	4.32	1.32	1.02	b
$PbSbO_3$	-0.56	0.23	2.78	1.32	0.44	a
$YCaO_3$	1.68	4.26	4.62	1.35	0.94	a
$BaTiO_3$	0.98	3.58	4.21	1.36	-0.26	None
$CaRhO_3$	-1.74	0.17	2.33	1.36	0.82	a,b
$BaHgO_3$	2.18	4.78	5.29	1.37	0.96	None
$NaSbO_3$	0.59	3.19	4.12	1.37	0.20	None
$NaOsO_3$	-0.38	0.17	2.79	1.38	0.54	None
$CaIrO_3$	-0.82	0.10	2.31	1.38	0.82	b
$BaAgO_3$	2.26	4.88	5.23	1.39	1.04	None
$SrHgO_3$	2.13	4.76	5.27	1.39	1.12	None
$KSbO_3$	0.86	3.49	4.39	1.40	0.16	None
$SrCrO_3$	-0.21	0.48	3.11	1.40	-0.16	a
$SrAgO_3$	2.15	4.78	4.84	1.40	1.16	None
$KBiO_3$	1.85	4.51	5.05	1.43	0.56	None
$GeTiO_3$	-0.47	0.17	2.84	1.43	0.20	a,b
$NaTaO_3$	-1.24	-0.04	2.26	1.43	-0.58	None
$SrPbO_3$	1.54	4.21	4.74	1.44	0.54	None
$MgYO_3$	2.65	5.34	5.19	1.46	1.16	None
$CaOsO_3$	-0.34	0.29	2.98	1.46	0.70	a
$BaMnO_3$	-0.74	-0.19	2.51	1.47	-0.08	a,b
$BaZnO_3$	2.38	5.09	5.14	1.48	0.66	None
$BaOsO_3$	-0.94	-0.43	2.28	1.48	0.46	a
$BaTlO_3$	2.05	4.77	5.02	1.49	0.74	None
$SrTlO_3$	2.03	4.75	5.06	1.49	0.88	None
$SrZnO_3$	2.41	5.13	5.15	1.49	0.74	None
$SiWO_3$	-0.74	-0.08	2.64	1.49	1.30	a
$LiGeO_3$	2.06	4.79	5.04	1.49	0.60	a
$MgScO_3$	2.73	5.36	5.23	1.50	0.90	None
$BaPbO_3$	1.73	4.46	4.89	1.50	0.40	None
$LiPbO_3$	2.33	5.07	5.10	1.51	1.28	b
$LiSbO_3$	-0.61	2.13	2.95	1.51	0.44	b
$SrAlO_3$	2.15	4.90	4.83	1.53	0.22	None

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$KPbO_3$	2.14	4.89	5.12	1.53	0.82	None
$SrGeO_3$	1.11	3.87	4.53	1.53	0.16	None
$CaAlO_3$	2.24	5.00	4.92	1.53	0.30	None
$LiTiO_3$	2.77	5.32	5.16	1.54	0.40	None
$AlLiO_3$	1.34	2.63	5.39	1.54	2.08	b
$KCdO_3$	2.61	5.39	5.24	1.54	1.28	a
$CaGeO_3$	1.09	3.87	4.31	1.55	0.16	None
$LaZnO_3$	2.37	5.16	5.10	1.55	0.44	None
$KSnO_3$	1.79	4.57	4.82	1.55	0.34	None
$LiSnO_3$	2.32	5.10	5.00	1.55	0.72	None
$BaCdO_3$	2.44	5.22	5.20	1.55	0.78	None
$LiTaO_3$	-1.92	-0.57	2.22	1.56	-0.32	b
$LaAsO_3$	-1.11	0.43	2.13	1.56	0.44	b
$NaAsO_3$	-0.69	0.36	2.12	1.57	0.52	b
$KCuO_3$	2.07	4.88	4.93	1.57	1.30	a
$LaIrO_3$	-0.88	0.25	2.12	1.57	0.78	b
$InReO_3$	-0.75	-0.61	2.12	1.57	0.46	a
$AlRhO_3$	-1.03	0.37	2.11	1.58	1.42	
$BaGaO_3$	2.15	4.97	4.95	1.59	0.20	None
$SrCdO_3$	2.26	5.09	5.14	1.59	0.92	None
$PbPdO_3$	0.64	3.46	4.02	1.59	1.14	a
$YCuO_3$	1.72	4.55	4.75	1.59	0.82	None
$PbHgO_3$	1.96	4.79	4.85	1.60	1.38	a
$CaSiO_3$	0.61	3.44	4.09	1.60	0.10	None
$SrGaO_3$	2.21	5.04	4.98	1.60	0.26	None
$BaSnO_3$	1.35	4.19	4.59	1.60	-0.08	None
$KZrO_3$	2.22	5.06	5.02	1.61	0.12	None
$ScOsO_3$	-0.64	-0.14	2.70	1.61	1.48	a
$LiZrO_3$	2.61	5.45	5.07	1.61	0.50	None
$SrSnO_3$	1.22	4.06	4.49	1.62	0.00	None
$CaAuO_3$	1.45	4.29	4.33	1.62	1.26	None
$KHfO_3$	2.15	5.00	4.96	1.62	0.12	None
$LiHfO_3$	2.50	5.35	5.06	1.62	0.52	None
$CaZnO_3$	2.21	5.08	5.17	1.63	0.88	a
$HgNiO_3$	-0.65	-0.17	2.69	1.63	1.40	a,b
$SrZrO_3$	1.30	4.16	4.54	1.63	-0.18	None
$CaGaO_3$	2.20	5.06	5.00	1.63	0.40	None
$LaTlO_3$	-0.71	2.13	2.06	1.63	0.70	b
$BaZrO_3$	1.36	4.23	4.57	1.64	-0.28	None
$NaSnO_3$	1.78	4.66	4.88	1.65	0.44	None
$CaTeO_3$	-1.68	0.10	2.04	1.65	0.60	b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$NaZrO_3$	2.19	5.07	5.03	1.66	0.24	None
$MgAlO_3$	2.04	4.95	4.91	1.67	0.54	None
$NaHfO_3$	2.13	5.03	4.98	1.67	0.24	None
$CaAgO_3$	1.79	4.69	4.54	1.67	1.30	None
$LaAgO_3$	1.77	4.68	4.45	1.68	0.96	b
$BaInO_3$	2.03	4.94	4.91	1.69	0.28	None
$PbAuO_3$	1.50	4.42	4.58	1.69	1.34	a,b
$BaScO_3$	2.25	5.18	4.97	1.70	0.22	None
$LaGaO_3$	1.98	4.91	4.92	1.70	-0.04	None
$YAlO_3$	1.93	4.85	4.79	1.70	0.14	None
$LaAlO_3$	2.00	4.93	4.80	1.70	-0.10	None
$YCdO_3$	-0.17	2.77	2.73	1.70	1.24	b
$BaHfO_3$	1.32	4.25	4.52	1.70	-0.26	None
$SrHfO_3$	1.24	4.18	4.47	1.71	-0.16	None
$LiTeO_3$	-0.49	2.44	2.64	1.71	0.74	b
$SrInO_3$	1.88	4.82	4.83	1.71	0.44	None
$AgTaO_3$	-0.99	-0.52	2.43	1.73	-0.04	a
$SrScO_3$	2.18	5.14	4.93	1.73	0.34	None
$LaAuO_3$	1.21	4.17	4.11	1.73	1.10	b
$CaYO_3$	1.50	4.46	4.55	1.74	0.58	None
$CaScO_3$	2.00	4.96	4.84	1.74	0.52	None
$CaCrO_3$	-0.02	0.46	3.44	1.74	-0.04	a
$SrYO_3$	1.58	4.55	4.57	1.74	0.46	None
$BaYO_3$	1.80	4.78	4.75	1.75	0.32	None
$LiBiO_3$	-0.29	2.70	3.05	1.76	1.00	b
$YGaO_3$	1.26	4.26	4.29	1.76	0.30	b
$PbZrO_3$	0.85	3.84	4.18	1.76	0.08	a
$PbLaO_3$	-2.58	-0.06	1.93	1.76	0.84	a,b
$LaScO_3$	1.65	4.64	4.44	1.76	0.08	None
$YCoO_3$	-0.79	2.21	3.16	1.77	0.60	a,b
$ScGaO_3$	-1.65	1.35	2.62	1.78	0.42	a,b
$ScZnO_3$	-0.79	-0.43	2.57	1.78	0.92	a,b
$ScTlO_3$	2.20	5.22	5.16	1.79	1.76	a
$AgOsO_3$	-1.28	0.35	1.89	1.80	1.10	b
$CaHfO_3$	0.76	3.81	3.95	1.82	0.02	b
$PbHfO_3$	0.93	3.99	4.25	1.83	0.10	a
$LaMgO_3$	2.19	5.25	4.86	1.83	0.34	None
$GaNbO_3$	-1.03	-0.63	2.44	1.84	0.08	a
$CaZrO_3$	0.66	3.72	3.77	1.84	0.02	b
$PbSnO_3$	0.85	3.92	4.12	1.84	0.28	b
$NaBiO_3$	0.92	4.02	4.25	1.86	0.72	a,b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$InAlO_3$	0.33	3.42	3.44	1.86	0.46	b
$NaYO_3$	2.01	5.11	4.81	1.87	0.86	a
$NaZnO_3$	2.47	5.58	5.26	1.88	1.22	a
$SrOsO_3$	-1.35	-0.92	1.81	1.88	0.54	a
$CaHgO_3$	1.57	4.70	4.83	1.89	1.32	b
$InTiO_3$	-2.33	-1.22	1.79	1.90	0.24	a,b
$AgZrO_3$	-2.83	-0.40	1.76	1.93	0.72	a,b
$CaVO_3$	0.00	-0.22	2.95	1.94	-0.14	a
$KMoO_3$	-0.18	-0.13	3.05	1.95	-0.22	None
$AgPtO_3$	-1.22	-0.93	2.24	1.95	1.70	a,b
$NaScO_3$	2.19	5.38	4.99	1.96	0.76	a
$GaTaO_3$	-1.35	-0.97	2.24	1.98	-0.04	a
$NaAuO_3$	1.24	4.50	4.49	2.03	1.54	a,b
$GaMoO_3$	-0.29	-0.49	2.78	2.03	0.30	a
$GaBO_3$	3.28	3.21	5.04	2.05	1.14	a,b
$InBaO_3$	-2.53	-1.52	1.64	2.05	1.60	a,b
$NaMoO_3$	-0.28	-0.31	2.96	2.05	-0.14	None
$YZnO_3$	1.74	5.03	4.54	2.06	0.76	None
$CaRuO_3$	-1.24	-0.10	1.62	2.07	0.66	a,b
$CaSnO_3$	0.36	3.65	3.64	2.07	0.16	b
$PbGeO_3$	-1.35	-1.15	2.14	2.07	0.30	a,b
$LaRuO_3$	-1.62	0.93	1.61	2.08	0.64	b
$PbVO_3$	-0.39	-0.63	2.71	2.11	0.04	a
$MgTiO_3$	-2.15	0.22	1.58	2.11	0.02	b
$ScAlO_3$	0.70	4.07	3.80	2.14	0.44	None
$BaAlO_3$	2.05	1.42	4.78	2.14	0.26	
$CaInO_3$	1.24	4.62	4.31	2.15	0.64	b
$AlAlO_3$	-1.12	1.45	1.53	2.16	1.14	b
$BaMoO_3$	-0.54	-0.72	2.66	2.16	-0.20	None
$InMoO_3$	-0.25	-0.46	2.95	2.18	0.26	None
$SrVO_3$	-0.19	-0.32	3.10	2.19	-0.26	None
$SrMoO_3$	-0.66	-0.88	2.55	2.20	-0.12	None
$AgMoO_3$	-0.27	-0.48	2.95	2.20	0.40	None
$SiBeO_3$	2.92	6.38	5.63	2.22	2.06	a,b
$PbYO_3$	-1.51	-1.45	2.01	2.22	0.60	a,b
$ScAgO_3$	-3.10	-1.26	1.46	2.23	1.48	a,b
$NaPbO_3$	1.05	4.51	4.41	2.24	1.00	a,b
$LaBaO_3$	-1.00	-1.12	2.35	2.24	1.38	a,b
$CaTlO_3$	1.05	4.53	4.14	2.25	1.12	b
$LiMoO_3$	0.04	-0.77	2.72	2.26	0.10	b
$BaSiO_3$	-2.68	-1.99	1.43	2.26	0.26	b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$LaVO_3$	-1.25	-1.30	2.19	2.27	-0.10	a
$InOsO_3$	-3.37	0.13	1.66	2.27	0.92	a,b
$NaCrO_3$	-1.00	-1.17	2.34	2.28	0.06	a,b
$LaCdO_3$	1.42	4.96	4.20	2.31	0.78	b
$BaVO_3$	-0.58	-0.79	2.76	2.32	-0.30	None
$PbMoO_3$	-0.73	-1.09	2.47	2.32	0.18	a
$ScCrO_3$	-1.62	-1.64	1.92	2.33	0.28	a,b
$AgBiO_3$	-1.64	-1.67	1.91	2.34	1.22	a,b
$YPtO_3$	-0.75	2.83	2.38	2.35	1.14	b
$ScSiO_3$	-0.55	-0.41	3.21	2.39	0.74	None
$BaCrO_3$	-1.65	-0.82	1.27	2.42	-0.14	a,b
$InNbO_3$	-1.11	-1.29	2.39	2.44	0.06	None
$YSnO_3$	-4.59	-1.60	1.24	2.45	0.88	b
$InZrO_3$	-3.22	-2.04	1.24	2.45	0.34	a,b
$LiLaO_3$	-2.71	-2.31	1.39	2.47	1.22	a,b
$ZrOsO_3$	-4.12	-0.54	1.20	2.49	1.44	a,b
$InPtO_3$	-1.80	-1.96	1.77	2.50	1.16	a,b
KWO_3	-1.20	-1.63	2.12	2.52	-0.32	None
$InTaO_3$	-1.35	-1.58	2.17	2.52	-0.16	None
$PbCuO_3$	0.77	4.54	4.31	2.54	1.10	a,b
$CaReO_3$	-1.67	-1.85	1.92	2.54	0.32	a
$LaReO_3$	-1.04	-1.57	2.23	2.58	0.56	a
$NaWO_3$	-1.33	-1.85	2.00	2.62	-0.26	None
$BiTiO_3$	-1.61	-2.00	1.89	2.66	0.42	a
$InWO_3$	-1.19	-1.76	2.13	2.66	0.18	a
$LaTiO_3$	-1.33	-1.86	2.06	2.68	0.02	None
$ZrBeO_3$	-3.96	-1.74	1.01	2.68	0.58	a,b
$LaBiO_3$	-0.92	3.01	1.99	2.70	0.82	b
$TeNiO_3$	-1.68	-2.12	1.84	2.73	1.28	a,b
$AgWO_3$	-1.22	-1.86	2.11	2.73	0.30	None
$GaWO_3$	-1.24	-1.90	2.08	2.75	0.20	a
$PbWO_3$	-1.98	-2.29	1.69	2.75	0.22	a
$BaLaO_3$	-0.29	3.70	3.12	2.76	0.40	b
$BaNbO_3$	-1.28	-1.91	2.09	2.77	-0.34	None
$LaInO_3$	0.16	4.20	3.24	2.81	0.20	b
$SrNbO_3$	-1.43	-2.13	1.92	2.82	-0.24	None
$GaAsO_3$	-3.92	-2.54	0.85	2.84	0.94	a,b
$PbGaO_3$	-2.16	-2.60	1.47	2.84	0.52	a,b
$YTiO_3$	-1.71	-2.27	1.81	2.85	0.22	a
$LaHfO_3$	-2.84	-2.96	0.83	2.86	0.16	None
$YBiO_3$	-4.11	-2.27	0.83	2.86	0.88	a,b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$ScCaO_3$	0.83	4.95	4.42	2.88	1.78	a,b
$YAgO_3$	0.47	4.58	3.29	2.88	1.44	b
$CaPbO_3$	-0.40	3.75	2.72	2.93	0.68	b
$PbNbO_3$	-1.37	-2.21	1.96	2.94	0.04	a
$YIrO_3$	-2.15	-1.94	0.74	2.95	1.06	b
$ZrAlO_3$	-3.56	0.07	0.74	2.95	0.50	b
$PbReO_3$	-2.30	-2.84	1.36	2.97	0.46	a,b
$NaNiO_3$	-1.91	-2.57	1.64	2.98	1.02	a,b
$YMoO_3$	-2.83	-3.04	1.18	2.99	0.68	a,b
$YInO_3$	-2.68	-0.23	0.70	2.99	0.48	b
$SrSiO_3$	-0.71	3.02	0.69	3.00	0.10	b
$CaNbO_3$	-1.54	-2.38	1.85	3.01	-0.06	a
$AgSnO_3$	-2.37	-2.96	1.31	3.03	0.92	a,b
$SrAsO_3$	-2.00	-2.88	1.37	3.03	0.28	b
$InNiO_3$	-0.89	3.39	3.37	3.05	0.90	a,b
$ScScO_3$	-4.92	-1.69	0.63	3.06	0.56	a,b
$KNiO_3$	-2.01	-2.76	1.56	3.09	1.04	a,b
$InAuO_3$	-4.63	-2.42	0.59	3.10	1.40	a,b
$LaSnO_3$	-2.92	0.89	0.55	3.14	0.46	b
$InSbO_3$	-4.05	0.32	1.42	3.14	0.58	a,b
$PbAgO_3$	0.43	4.83	4.23	3.17	1.36	a,b
$CaPdO_3$	-1.53	1.38	0.48	3.21	1.00	a,b,c
$LaHgO_3$	0.24	4.68	4.01	3.21	1.12	b
$PbTaO_3$	-1.91	-2.83	1.61	3.21	0.18	a
$LaSbO_3$	-2.66	1.83	1.15	3.26	0.64	b
$YAuO_3$	-0.37	4.15	2.84	3.28	1.56	b
$YOsO_3$	-0.51	0.02	4.55	3.30	1.08	b
$YBaO_3$	-2.26	-1.82	2.73	3.32	1.20	b
$InScO_3$	-2.69	-3.52	1.05	3.34	0.52	a,b
$NaSiO_3$	-1.95	0.27	4.86	3.36	0.38	b
$PdNiO_3$	-2.28	-3.26	1.34	3.37	1.52	a,b
$ZrVO_3$	-4.43	-4.03	0.31	3.38	0.78	a,b
$KAsO_3$	-4.22	-2.11	0.30	3.39	0.56	b
$InRuO_3$	-2.76	-3.64	0.99	3.40	0.88	a,b
$InRhO_3$	-2.78	-3.69	0.97	3.43	0.94	a,b
$InHfO_3$	-2.47	2.21	0.77	3.45	0.34	b
$ScTiO_3$	-2.38	-3.46	1.25	3.48	0.26	a,b
$YZrO_3$	-3.85	-4.22	0.51	3.50	0.54	a,b
$LaLaO_3$	-3.29	-0.98	0.17	3.52	0.44	b
$InIrO_3$	-1.79	2.96	2.92	3.52	1.02	a,b
$LaYO_3$	-0.88	3.87	2.14	3.52	0.26	b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$InCrO_3$	-2.89	-3.87	0.88	3.53	0.26	a,b
$ScCoO_3$	-2.63	2.17	2.40	3.57	0.76	a,b
$RuNiO_3$	-2.47	-3.63	1.18	3.58	1.54	a,b
$LaPbO_3$	-1.71	3.12	3.85	3.60	0.66	b
$YSbO_3$	-2.49	-3.66	1.17	3.60	1.08	a,b
$GaOsO_3$	-4.66	-4.82	0.05	3.64	0.98	a,b
$PbAsO_3$	-3.18	-4.39	0.65	3.80	0.56	a,b
$YTlO_3$	-3.26	-0.60	-0.13	3.82	1.00	b
$YRuO_3$	-3.14	-2.00	-0.15	3.84	1.04	b
$YHfO_3$	-3.84	-2.84	-0.22	3.91	0.52	b
$AlSiO_3$	-1.44	3.77	2.77	3.98	1.04	b
$ScBeO_3$	-5.48	-4.92	-0.30	3.99	0.96	a,b
$YNbO_3$	-3.38	-4.60	0.62	3.99	0.38	a,b
$KGeO_3$	-3.45	-4.99	0.23	3.99	0.42	a,b
$CaAsO_3$	-1.60	-3.21	2.03	4.01	0.42	b
$MgAuO_3$	-0.97	4.28	2.78	4.02	1.38	b
$ZrNiO_3$	-2.07	3.23	2.86	4.06	1.08	a,b
$ZrLiO_3$	-5.56	-5.13	-0.38	4.07	0.98	a,b
$YAsO_3$	-3.28	2.10	0.42	4.14	0.74	b
$AgSiO_3$	-3.63	-5.33	0.07	4.17	0.98	a,b
$SrLaO_3$	-2.26	3.31	2.31	4.34	0.62	b
$PbCdO_3$	-3.81	-5.49	0.14	4.40	1.20	a,b
$ZrCoO_3$	-3.64	2.02	1.96	4.43	1.02	a,b
$CaLaO_3$	-1.57	2.56	-0.76	4.45	0.64	b
YYO_3	-4.41	-1.19	-0.80	4.49	0.56	b
$InCoO_3$	-3.42	2.32	2.11	4.51	0.80	a,b
$GaPtO_3$	-7.12	-4.32	-0.84	4.53	1.30	a,b
$AgAsO_3$	-3.95	-5.75	0.01	4.54	1.12	a,b
$MgNiO_3$	-2.48	3.29	2.70	4.54	0.84	a,b
$BaAsO_3$	-3.08	-3.79	2.00	4.56	0.22	b
$ZrZnO_3$	-6.23	-6.12	-0.87	4.56	0.86	a,b
$LaCrO_3$	-0.27	-0.62	-0.91	4.60	-0.20	c
$PbTlO_3$	-1.31	4.63	3.47	4.71	1.16	a,b
$GaHfO_3$	-7.11	-5.29	-1.05	4.74	0.56	a,b
$InAgO_3$	-1.34	4.64	3.47	4.75	1.36	a,b
$ZrNbO_3$	-6.37	-6.79	-1.07	4.76	0.64	a,b
$ScZrO_3$	-5.56	-6.74	-0.73	4.78	0.34	a,b
$InSnO_3$	-4.16	1.86	1.71	4.79	0.46	a,b
$InGeO_3$	-5.09	0.97	1.14	4.84	0.46	a,b
$TiBeO_3$	-3.68	-5.93	0.18	4.88	0.82	a,b
$MgBiO_3$	-3.36	2.83	0.51	4.96	0.74	b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$ZrCuO_3$	-7.07	-0.87	-0.07	4.97	1.08	a,b
$PtNiO_3$	-3.81	-6.17	0.07	5.02	1.86	a,b
$YPbO_3$	-3.36	2.91	0.47	5.04	1.36	b
$YSrO_3$	-3.83	-6.22	0.05	5.04	1.08	a,b
$ScHgO_3$	-3.91	-6.37	-0.01	5.13	2.00	a,b
$MgOsO_3$	-1.29	-1.11	-1.45	5.14	1.06	b,c
$KCrO_3$	-4.61	-7.07	-0.69	5.16	0.08	a,b
$NaReO_3$	-3.27	-0.74	-1.51	5.20	-0.04	a,c
$MgInO_3$	-4.75	-7.87	-1.40	5.24	1.02	a,b
$GeNiO_3$	-4.05	-6.63	-0.13	5.28	0.98	a,b
$MgCuO_3$	-2.01	4.51	-0.66	5.29	1.08	b
$MgZrO_3$	-5.07	-2.90	-1.62	5.31	0.14	b
$PbInO_3$	-1.78	4.77	3.31	5.32	0.68	a,b
$AgHfO_3$	-2.14	4.43	3.09	5.34	0.72	a,b
$CaMoO_3$	-0.44	-1.48	-1.70	5.39	0.44	b,c
$InAsO_3$	-4.55	2.09	0.54	5.40	0.82	b
$InVO_3$	-4.87	-7.36	-0.73	5.40	0.20	a,b
$MgPbO_3$	-4.08	-7.63	-1.73	5.42	1.20	a,b
$MgSiO_3$	-1.82	1.73	-1.76	5.45	0.28	b
$InTeO_3$	-5.05	-7.68	-0.88	5.57	0.80	a,b
$MgHfO_3$	-5.10	-8.63	-1.82	5.58	0.40	a,b
$GaCrO_3$	-5.14	-7.85	-0.95	5.66	0.32	a,b
$YSiO_3$	-2.94	-3.99	2.91	5.66	0.72	b
$MgTlO_3$	-5.20	-8.13	-1.19	5.71	1.52	a,b
$MgSbO_3$	-5.19	-8.11	-1.18	5.71	0.72	a,b
$MgGeO_3$	-4.65	2.38	1.71	5.80	0.34	b
YWO_3	-1.33	-1.48	-2.16	5.85	0.78	b,c
$HfTiO_3$	-4.63	-7.74	-0.61	5.90	0.84	a,b
$LiAsO_3$	-3.26	3.89	1.03	5.92	0.72	b
$MgSnO_3$	-5.55	-8.62	-1.44	5.95	0.32	a,b
$ScInO_3$	-9.63	-6.10	-2.26	5.95	0.70	a,b
$TiNiO_3$	-4.69	-7.86	-0.66	5.97	1.04	a,b
$MgAsO_3$	-5.53	-9.51	-2.30	5.99	0.76	a,b
$NaGeO_3$	-2.81	4.44	4.88	6.02	0.38	b
$LaTeO_3$	-5.42	-4.98	-2.36	6.05	0.82	b
$GaTeO_3$	-9.01	-7.79	-2.37	6.06	0.92	a,b
$GaSbO_3$	-5.45	1.91	1.19	6.13	0.66	a,b
$BaReO_3$	-1.08	-1.43	-2.46	6.15	0.10	c
$NbAlO_3$	-5.70	-8.83	-1.41	6.19	0.62	a,b
$GaAlO_3$	-8.23	-0.79	-0.53	6.21	0.78	a,b
$CaCdO_3$	-5.73	-8.88	-1.43	6.22	1.14	a,b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$GaRuO_3$	-5.73	-8.89	-1.44	6.22	1.06	a,b
$AlNbO_3$	-9.52	-7.83	-2.59	6.28	0.84	a,b
$MgHgO_3$	-2.58	4.49	-2.66	6.35	1.72	a,b
$YTeO_3$	-5.06	-8.56	-0.97	6.37	1.38	a,b
$MgGaO_3$	-2.87	4.79	4.92	6.42	0.72	b
$SrReO_3$	-1.22	-1.59	-2.74	6.43	0.16	c
$YBeO_3$	-5.70	-5.88	-2.75	6.44	0.72	b
$SiTiO_3$	-8.20	-10.31	-2.59	6.49	0.62	a,b
$NaCuO_3$	-6.05	-9.46	-1.70	6.53	1.32	a,b
$InTlO_3$	-6.10	-9.54	-1.74	6.57	1.38	a,b
$ScBiO_3$	-5.31	-9.03	-1.17	6.63	1.56	a,b
$LaBeO_3$	-6.14	-5.25	-3.02	6.71	0.56	b
$LaSiO_3$	-1.41	-2.89	-3.05	6.74	0.48	b,c
$LaNbO_3$	-1.93	-2.91	-3.12	6.81	0.16	b,c
$AgPbO_3$	-4.92	3.14	1.68	6.83	1.48	a,b
$ZrAgO_3$	-10.56	-8.61	-3.18	6.87	1.58	a,b
$LaOsO_3$	-2.77	-2.57	-3.28	6.97	0.80	b,c
$GaSnO_3$	-10.51	-9.22	-3.29	6.98	0.60	a,b
$SiSiO_3$	-6.65	-10.50	-2.18	7.09	1.04	a,b
$BaWO_3$	-1.44	-2.03	-3.40	7.09	-0.16	c
$YLaO_3$	-7.32	-4.87	-3.43	7.12	0.78	b
$YMgO_3$	-3.24	5.14	0.43	7.15	0.68	b
$IrNiO_3$	-5.82	-10.01	-1.60	7.18	2.00	a,b
$PbBeO_3$	-6.82	-10.81	-2.33	7.25	1.18	a,b
$PbSiO_3$	-6.88	-10.92	-2.38	7.31	0.48	a,b
$AgGeO_3$	-4.42	4.13	2.10	7.32	0.90	a,b
$SrWO_3$	-1.57	-2.24	-3.72	7.41	-0.08	c
$InBiO_3$	-5.70	2.95	1.32	7.42	0.90	a,b
$ZrPtO_3$	-11.17	-10.19	-3.78	7.47	1.54	a,b
$ZrGaO_3$	-6.12	-10.57	-1.84	7.50	0.64	a,b
$MoNiO_3$	-6.21	-10.74	-1.92	7.59	1.30	a,b
$CaWO_3$	-1.81	-2.39	-3.94	7.63	0.10	b,c
$MgTeO_3$	-6.47	2.46	-3.58	7.70	0.70	b
$KSiO_3$	-5.36	3.59	-1.55	7.71	0.56	b
$CaBeO_3$	-7.32	-11.68	-2.73	7.72	0.98	a,b
$ZrAuO_3$	-6.39	-11.10	-2.07	7.80	1.72	a,b
$AlVO_3$	-2.12	-2.17	-4.13	7.82	0.96	b,c
$GaZrO_3$	-7.42	-11.87	-2.81	7.82	0.56	a,b
$InSiO_3$	-9.50	-0.44	-0.97	7.83	0.58	a,b
$ZrScO_3$	-6.43	-11.17	-2.11	7.84	0.50	a,b
$MgMoO_3$	-0.88	-7.40	-4.17	7.86	0.42	a,b,c

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$MgLaO_3$	-5.91	3.31	-3.96	7.99	1.30	b
$AlBeO_3$	-8.41	-8.25	-4.37	8.06	1.60	b
$LiWO_3$	-2.81	-2.75	-4.43	8.12	0.00	b,c
$InPbO_3$	-6.31	3.08	1.10	8.15	1.08	a,b
$MgBeO_3$	-7.89	-12.69	-3.20	8.26	1.14	a,b
$InCdO_3$	-7.92	-12.75	-3.22	8.30	1.38	a,b
$BaTaO_3$	-2.05	-2.84	-4.73	8.42	0.04	c
$AlIrO_3$	-12.19	-13.24	-4.86	8.55	1.54	a,b
$GaCuO_3$	-8.28	-13.38	-3.51	8.63	1.44	a,b
$MgVO_3$	-1.75	-1.04	-5.00	8.69	0.02	b,c
$SrTaO_3$	-2.15	-3.03	-5.06	8.75	0.10	c
$LaTaO_3$	-2.87	-3.34	-5.07	8.76	0.06	b,c
$NaHgO_3$	-5.11	4.95	5.35	8.83	1.60	b
$MgNbO_3$	-1.36	-8.87	-5.16	8.85	0.48	a,b,c
$LaCaO_3$	-5.62	4.48	-1.09	8.87	0.68	b
$LaSrO_3$	-6.12	3.99	-2.89	8.87	0.78	b
$NbNiO_3$	-7.44	-13.08	-2.94	8.92	1.14	a,b
$CaTaO_3$	-2.15	-3.14	-5.31	9.00	0.16	c
$LaZrO_3$	-2.60	-2.93	-5.45	9.14	0.14	b,c
$AlCoO_3$	-7.51	-7.78	-5.55	9.24	1.08	a,b
$AlBaO_3$	-9.01	-14.67	-4.11	9.33	2.54	a,b
$ZrSbO_3$	-7.83	-13.83	-3.26	9.34	1.16	a,b
$NaBeO_3$	-9.29	-15.16	-4.34	9.59	1.30	a,b
$OsNiO_3$	-8.12	-14.38	-3.50	9.65	1.70	a,b
$BaBeO_3$	-9.36	-15.28	-4.40	9.66	0.96	a,b
$YTaO_3$	-4.24	-5.75	-6.07	9.76	0.44	b
$MgWO_3$	-1.60	-10.15	-6.17	9.86	0.42	a,b,c
$GaAgO_3$	-9.71	-15.90	-4.68	9.99	1.54	a,b
$GaMgO_3$	-9.83	-16.11	-4.78	10.10	1.32	a,b
$AlPtO_3$	-12.43	-9.50	-6.45	10.14	1.70	b
$MgCdO_3$	-6.83	4.71	4.84	10.31	1.52	b
$LaMoO_3$	-5.53	-4.02	-6.83	10.52	0.54	b,c
$SiHfO_3$	-10.64	-17.54	-5.44	10.87	0.76	a,b
$ZrYO_3$	-15.82	-17.27	-7.21	10.90	0.68	a,b
$AlNiO_3$	-8.98	3.29	-3.20	11.05	1.16	b
$MgTaO_3$	-1.96	-11.74	-7.37	11.06	0.38	a,b,c
$AlTaO_3$	-5.12	-7.90	-7.41	11.10	0.56	b,c
$InHgO_3$	-7.87	4.48	0.77	11.12	1.60	a,b
$ZrBiO_3$	-9.57	-17.15	-4.71	11.21	1.24	a,b
$AlMgO_3$	-1.35	-6.50	-7.77	11.46	0.98	b
$InLiO_3$	-11.28	-18.66	-5.96	11.47	1.18	a,b

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Formula	ΔG_{OH} (eV)	ΔG_{O} (eV)	ΔG_{OOH} (eV)	η_{OER} (V)	ΔE_{hull} (eV)	warnings
$YLiO_3$	-11.30	-18.70	-5.98	11.49	1.06	a,b
$GaGeO_3$	-11.31	-18.73	-5.99	11.51	0.66	a,b
$ZrBO_3$	-17.60	-18.02	-8.10	11.79	1.06	a,b
$NbBeO_3$	-11.97	-19.88	-6.52	12.13	0.78	a,b
$ReNiO_3$	-10.46	-18.83	-5.44	12.16	1.86	a,b
$InMgO_3$	-8.39	5.35	0.74	12.51	0.96	a,b
$SiNiO_3$	-10.90	-19.68	-5.81	12.64	1.58	a,b
$VBeO_3$	-12.52	-20.85	-6.97	12.65	0.92	a,b
$WNiO_3$	-10.93	-19.72	-5.83	12.66	1.58	a,b
$NbGeO_3$	-12.61	-21.02	-7.05	12.74	0.86	a,b
$AlWO_3$	-8.47	-2.15	-9.68	13.37	1.00	a,b,c
$GaBiO_3$	-13.53	-22.64	-7.80	13.61	1.08	a,b
$AlCuO_3$	-10.83	4.06	-6.63	13.66	1.86	b
$CaLiO_3$	-13.90	-23.29	-8.10	13.96	1.24	a,b
$GaPbO_3$	-14.19	-23.80	-8.34	14.23	1.06	a,b
$AlMoO_3$	-9.77	-9.07	-10.61	14.30	1.08	b,c
$AlZnO_3$	-14.65	-25.05	-9.17	14.66	1.24	a,b
$SiGeO_3$	-14.70	-24.70	-8.75	14.72	1.16	a,b
$AlAuO_3$	-14.47	-10.56	-11.87	15.56	1.94	b
$LaBO_3$	-14.27	-14.32	-11.91	15.60	0.60	b
$InBO_3$	-14.77	-27.95	-12.00	15.69	1.04	a,b
$AlGeO_3$	-14.36	-14.76	-12.26	15.95	1.20	b
$MgBO_3$	-15.49	-13.22	-12.28	15.97	1.06	b,c
$CaCsO_3$	-16.36	4.13	-13.04	19.26	1.68	b
$AlHfO_3$	-15.70	-13.63	-16.83	20.52	0.68	b,c
$ZrLaO_3$	-22.21	-37.94	-14.88	21.83	0.90	a,b
$MgCsO_3$	-23.23	-40.43	-16.42	22.78	1.86	a,b
$SiAlO_3$	-25.02	-42.89	-17.17	24.49	1.38	a,b
$BaBaO_3$	1.30	-24.89	4.31	27.97	0.88	b
$CaBaO_3$	1.02	-27.19	4.33	30.28	1.40	b
$SrBaO_3$	1.04	-29.06	4.35	32.18	1.12	b
$SiPbO_3$	-37.55	-64.99	-27.39	36.37	1.74	a,b
$BaCsO_3$	-33.40	4.39	-9.67	36.56	1.36	a,b

a: One or more runs did not converge or failed in Quantum Espresso, missing adsorbates are reconstructed from successful runs using scaling

b: Changes in atomic positions of greater than 5.5 Å found in the slab or adsorbate during optimization, typically indicates structural instability

c: OH or OOH bond length changes significantly during optimization, indicates bond-dissociation of the adsorbate

d: Adsorbate migration from initial active site greater than 4 Å

4 Hydrogen evolution data

Data include for hydrogen evolution in the table below also includes vacancy formation energies. In addition to the repeated relevant warnings regarding surface and adsorbate site migration, an additional warning is indicated if the vacancy formation energy is exergonic at the limiting potential of hydrogen evolution.

Formula	ΔG_{H*-M} (eV)	ΔG_{H*-O} (eV)	η_{HER} (V)	ΔE_{hull} (eV)	$\Delta G_{vacancy}$ (eV)	warnings
$GaNbO_3$	0.01	0.06	-0.01	0.08	2.01	None
$SrNiO_3$	-0.01	-2.55	-0.01	0.64	-4.37	e
$LaTiO_3$	-0.02	1.89	-0.02	0.02	3.65	None
$GaTaO_3$	-0.03	1.21	-0.03	-0.04	2.43	None
$NaTaO_3$	-0.04	1.62	-0.04	-0.58	3.60	None
$LaTaO_3$	-1.08	-0.06	-0.06	0.06	1.58	None
$SrPdO_3$	0.08	-2.41	-0.08	0.96	-3.38	b,e
$NaOsO_3$	-0.97	0.09	-0.09	0.54	-0.57	None
$BaRhO_3$	-0.11	-1.92	-0.11	0.60	-2.30	e
$SrTiO_3$	2.36	-0.12	-0.12	-0.24	1.80	None
$BaNbO_3$	-0.13	1.61	-0.13	-0.34	3.75	None
$PbPdO_3$	0.14	-2.45	-0.14	1.14	-3.06	b,e
$SrMoO_3$	-0.15	1.13	-0.15	-0.12	2.83	None
$CaTiO_3$	2.61	0.15	-0.15	-0.12	1.93	None
$SrSiO_3$	0.57	0.15	-0.15	0.10	1.30	None
$LaPdO_3$	0.17	-1.47	-0.17	0.72	-1.77	e
$CaZrO_3$	2.22	0.20	-0.20	0.02	2.50	b
$BaGeO_3$	0.21	-1.54	-0.21	0.02	-4.07	e
$SrVO_3$	0.56	0.23	-0.23	-0.26	1.55	None
$GaMoO_3$	0.30	0.25	-0.25	0.30	0.81	None
$PbNbO_3$	-0.26	0.88	-0.26	0.04	2.18	None
$LaCoO_3$	0.27	-1.85	-0.27	0.30	-1.78	b,e
$SrNbO_3$	-0.29	1.77	-0.29	-0.24	3.67	None
$NaMoO_3$	0.33	0.54	-0.33	-0.14	1.20	None
$BaIrO_3$	-0.37	-0.63	-0.37	0.62	-0.64	e
$LaNbO_3$	-0.63	0.40	-0.40	0.16	1.90	None
$LaRuO_3$	-0.40	-2.57	-0.40	0.64	-1.29	b
$LaRhO_3$	-0.41	-1.83	-0.41	0.68	-1.33	b
$CaNbO_3$	-0.43	1.84	-0.43	-0.06	3.52	None
$CaVO_3$	0.87	0.46	-0.46	-0.14	1.88	None
$NaNbO_3$	0.46	0.73	-0.46	-0.32	2.85	None
$BaPtO_3$	-0.47	-1.52	-0.47	0.78	-1.80	e
$SrIrO_3$	-0.47	-2.63	-0.47	0.70	-0.10	b
$NaTeO_3$	0.48	-2.01	-0.48	0.48	-3.17	b,e
$SrAuO_3$	0.49	-1.94	-0.49	1.12	-2.51	e

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Formula	ΔG_{H*-M} (eV)	ΔG_{H*-O} (eV)	η_{HER} (V)	ΔE_{hull} (eV)	$\Delta G_{vacancy}$ (eV)	warnings
$LaNiO_3$	0.50	-1.43	-0.50	0.36	-1.91	e
$LaPtO_3$	-0.50	-0.73	-0.50	0.84	-0.54	e
$SrSbO_3$	-0.51	-1.29	-0.51	0.18	-2.14	b,e
$LaGeO_3$	-0.67	-0.52	-0.52	0.28	-1.64	b,e
$LaPbO_3$	0.52	-2.13	-0.52	0.66	-3.25	b,e
$CaAuO_3$	0.53	-1.81	-0.53	1.26	-2.51	e
$BaTiO_3$	2.60	-0.54	-0.54	-0.26	1.25	None
$BaAuO_3$	0.55	-2.01	-0.55	1.02	-2.64	e
$GaWO_3$	-0.56	1.14	-0.56	0.20	1.24	None
$NaWO_3$	-0.62	1.51	-0.62	-0.26	1.79	None
$LaAuO_3$	0.64	-1.13	-0.64	1.10	-1.83	e
$LaSiO_3$	-0.66	1.19	-0.66	0.48	2.64	None
$LaHfO_3$	-0.98	-0.66	-0.66	0.16	2.47	None
$NaSbO_3$	0.67	-0.76	-0.67	0.20	-1.63	e
$SrBiO_3$	0.68	-1.87	-0.68	0.42	-3.10	b,e
$LaSnO_3$	-0.69	-2.20	-0.69	0.46	-1.58	b,e
$BaSbO_3$	-0.69	-1.77	-0.69	0.04	-2.35	b,e
$LaZrO_3$	-0.70	-1.00	-0.70	0.14	2.51	b
$BaBiO_3$	0.72	-1.56	-0.72	0.28	-2.80	e
$LaHgO_3$	0.76	-2.33	-0.76	1.12	-3.60	b,e
$PbHfO_3$	2.34	0.77	-0.77	0.10	2.08	None
$SrReO_3$	-1.14	0.78	-0.78	0.16	0.27	None
$CaBiO_3$	0.79	-2.28	-0.79	0.68	-3.20	b,e
$BaReO_3$	-1.03	0.79	-0.79	0.10	0.53	None
$CaSnO_3$	0.86	-1.98	-0.86	0.16	-1.93	b,e
$BaBO_3$	1.62	0.86	-0.86	1.02	2.45	b
$CaBaO_3$	2.15	-0.88	-0.88	1.40	-2.01	e
$CaSiO_3$	1.06	0.89	-0.89	0.10	1.99	None
$SrGeO_3$	0.90	-1.26	-0.90	0.16	-2.99	e
$BaTaO_3$	-0.90	2.25	-0.90	0.04	4.04	None
$SrBO_3$	1.56	0.92	-0.92	0.96	2.46	None
$CaPbO_3$	1.01	-4.14	-1.01	0.68	-5.13	b,e
$SrWO_3$	-1.02	1.79	-1.02	-0.08	3.26	None
$SrTaO_3$	-1.02	2.38	-1.02	0.10	3.83	None
$CaTaO_3$	-1.03	1.22	-1.03	0.16	3.60	b
$PbSnO_3$	1.04	-1.56	-1.04	0.28	-1.22	e
$SrSnO_3$	1.22	-1.11	-1.11	0.00	-0.88	e
$BaSnO_3$	1.28	-1.16	-1.16	-0.08	-0.90	e
$SrAgO_3$	1.16	-2.23	-1.16	1.16	-3.42	e
$LaTlO_3$	-1.17	-3.51	-1.17	0.70	-5.53	b,e
$BaHgO_3$	1.18	-2.04	-1.18	0.96	-3.33	e

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Formula	ΔG_{H*-M} (eV)	ΔG_{H*-O} (eV)	η_{HER} (V)	ΔE_{hull} (eV)	$\Delta G_{vacancy}$ (eV)	warnings
$BaAgO_3$	1.19	-2.30	-1.19	1.04	-3.53	e
$SrHgO_3$	1.20	-1.97	-1.20	1.12	-3.31	e
$SrZrO_3$	2.49	1.20	-1.20	-0.18	3.52	None
$BaCuO_3$	1.23	-2.27	-1.23	0.82	-3.83	e
$CaHgO_3$	1.24	-2.11	-1.24	1.32	-5.91	b,e
$LaCuO_3$	1.26	-1.54	-1.26	0.54	-2.35	e
$CaCuO_3$	1.26	-2.14	-1.26	0.96	-3.70	e
$LaInO_3$	1.27	-3.74	-1.27	0.20	-3.42	b,e
$NaBiO_3$	1.29	-2.66	-1.29	0.72	-4.17	b,e
$GaAsO_3$	-4.34	-1.31	-1.31	0.94	-3.20	b,e
$LaAgO_3$	1.31	-1.41	-1.31	0.96	-2.49	e
$SrPbO_3$	1.34	-2.58	-1.34	0.54	-3.64	b,e
$SrHfO_3$	2.41	1.37	-1.37	-0.16	3.65	None
$BaZrO_3$	2.54	1.37	-1.37	-0.28	3.73	None
$BaTlO_3$	1.40	-2.18	-1.40	0.74	-4.04	e
$SrTeO_3$	1.54	-1.42	-1.42	0.38	-1.14	b,e
$SrTlO_3$	1.42	-2.37	-1.42	0.88	-4.20	b,e
$LaAsO_3$	-1.43	-2.60	-1.43	0.44	-2.65	b,e
$NaPbO_3$	1.45	-3.62	-1.45	1.00	-5.20	b,e
$LaAlO_3$	2.56	-1.50	-1.50	-0.10	-0.45	e
$BaPbO_3$	1.51	-2.09	-1.51	0.40	-3.24	e
$BaHfO_3$	2.44	1.60	-1.60	-0.26	3.87	None
$NaSiO_3$	2.20	-1.61	-1.61	0.38	-3.75	e
$BaAsO_3$	-1.67	-1.95	-1.67	0.22	-5.18	b,e
$CaAsO_3$	-1.67	-4.53	-1.67	0.42	-5.26	b,e
$CaInO_3$	1.70	-3.30	-1.70	0.64	-4.57	b,e
$NaSnO_3$	1.75	-2.20	-1.75	0.44	-3.12	e
$LaSbO_3$	1.85	-1.82	-1.82	0.64	-1.12	b,e
$SrInO_3$	1.83	-2.53	-1.83	0.44	-3.84	b,e
$LaZnO_3$	1.99	-1.83	-1.83	0.44	-3.19	e
$SrCdO_3$	1.84	-2.32	-1.84	0.92	-3.79	e
$LaIrO_3$	-1.87	-3.02	-1.87	0.78	-0.86	b
$BaInO_3$	1.89	-2.36	-1.89	0.28	-3.64	e
$LaCdO_3$	1.90	-2.27	-1.90	0.78	-4.80	b,e
$CaAlO_3$	2.56	-1.92	-1.92	0.30	-2.65	e
$LaLaO_3$	-1.92	-5.39	-1.92	0.44	-5.32	b,e
$LaBiO_3$	1.93	-2.63	-1.93	0.82	-1.42	b,e
$LaGaO_3$	2.08	-1.96	-1.96	-0.04	-1.85	e
$BaSiO_3$	-1.98	-8.13	-1.98	0.26	-5.41	b
$BaGaO_3$	2.00	-2.23	-2.00	0.20	-3.45	e
$CaRhO_3$	-2.00	-4.21	-2.00	0.82	-4.13	b,e

Continued on next page

Formula	ΔG_{H*-M} (eV)	ΔG_{H*-O} (eV)	η_{HER} (V)	ΔE_{hull} (eV)	$\Delta G_{vacancy}$ (eV)	warnings
$SrAlO_3$	2.46	-2.00	-2.00	0.22	-2.67	e
$LaYO_3$	2.01	-3.86	-2.01	0.26	-3.43	b,e
$CaLaO_3$	2.05	-4.41	-2.05	0.64	-4.72	b,e
$BaAlO_3$	2.30	-2.10	-2.10	0.26	-2.99	e
$NaTiO_3$	-2.31	-2.11	-2.11	0.18	-2.99	e
$NaHfO_3$	2.84	-2.11	-2.11	0.24	-2.34	e
$SrGaO_3$	2.12	-2.17	-2.12	0.26	-3.41	e
$SrBaO_3$	2.17	-7.71	-2.17	1.12	-2.75	b
$NaZrO_3$	2.93	-2.18	-2.18	0.24	-2.76	e
$CaGaO_3$	2.18	-2.22	-2.18	0.40	-3.74	e
$NaAsO_3$	-2.22	-3.94	-2.22	0.52	-4.85	b,e
$SrScO_3$	2.87	-2.22	-2.22	0.34	-3.26	e
$BaScO_3$	2.82	-2.24	-2.24	0.22	-3.18	e
$LaScO_3$	2.61	-2.30	-2.30	0.08	-1.69	b,e
$SrLaO_3$	2.31	-2.94	-2.31	0.62	-4.24	b,e
$BaYO_3$	2.59	-2.36	-2.36	0.32	-3.32	e
$CaYO_3$	2.40	-3.47	-2.40	0.58	-4.22	b,e
$SrYO_3$	2.42	-2.73	-2.42	0.46	-3.69	b,e
$BaLaO_3$	2.45	-2.48	-2.45	0.40	-3.89	b,e
$LaMgO_3$	2.71	-2.55	-2.55	0.34	-3.97	e
$CaScO_3$	2.77	-2.56	-2.56	0.52	-3.68	b,e
$NaLaO_3$	2.88	-2.60	-2.60	0.90	-4.95	b,e
$GaAlO_3$	-3.06	-9.47	-3.06	0.78	-9.50	b,e
$LaTeO_3$	-8.29	-4.47	-4.47	0.82	-5.06	b,e
$GaCuO_3$	-5.69	-9.81	-5.69	1.44	-8.31	b,e
$LaBeO_3$	-8.83	-9.58	-8.83	0.56	-9.92	b,e
$GaGeO_3$	-9.43	-10.17	-9.43	0.66	-9.22	b,e
$LaBO_3$	-13.51	-19.39	-13.51	0.60	-18.55	b,e
$BaCsO_3$	-18.42	-57.77	-18.42	1.36	-17.84	b

b: Changes in atomic positions of greater than 5.5 Å found in the slab or adsorbate during optimization, typically indicates structural instability

d: Adsorbate migration from initial active site greater than 4 Å

e: Vacancy formation energy is exergonic at HER limiting potential

5 PDOS data

We tabulate descriptors from the projected-density of states of the BO_2-terminated (100) ABO_3 perovskite surfaces used to generate Figures 5-7 in the main text. Included are the d, t_{2g} and e_g filling descriptors, the p-band centers, and the population of d-states at the Fermi level. The projected densities of states are determined via the ase-espresso code,[5] and the centers are defined as:

$$x\text{-center} = \frac{\int_{-\infty}^{\infty} \epsilon n_x(\epsilon)\, d\epsilon}{\int_{-\infty}^{\infty} n_x(\epsilon)\, d\epsilon} \tag{2}$$

where n_x is the projected density of states corresponding to the respective orbital (e.g. d, p, e_g, t_{2g}, etc.). The filling values are the projected densities of states integrated with respect to energy up to the fermi level, i.e.

$$x\text{-filling} = \int_{-\infty}^{\epsilon_{fermi}} n_x(\epsilon)\, d\epsilon \tag{3}$$

Formula	d-center (eV)	d-filling	e_g-filling	t_{2g}-filling	p-center (eV)	p-filling	d-states at E_f
$SrTiO_3$	1.68	2.02	1.00	1.02	-1.77	5.04	0.00
$YInO_3$	-13.27	9.84	3.93	5.92	-1.78	4.89	0.00
KVO_3	-0.38	3.39	1.45	1.94	-2.15	4.59	0.05
$CaTaO_3$	-0.45	3.27	1.14	2.12	-4.68	4.80	1.25
$SrWO_3$	-1.05	4.27	1.20	3.07	-4.23	4.84	1.36
$LaPtO_3$	-1.81	8.24	2.61	5.63	-2.07	4.73	1.01
$CaInO_3$	-12.57	9.83	3.92	5.92	-0.74	4.90	0.05
$BaCdO_3$	-6.42	9.72	3.80	5.91	-0.46	4.65	0.12
$YCuO_3$	-2.56	9.17	3.29	5.88	-1.30	4.69	0.47
$BaAgO_3$	-3.19	9.23	3.38	5.84	-0.61	4.60	0.43
$KCrO_3$	-1.24	4.38	1.56	2.82	-2.08	4.61	1.66
$KZrO_3$	3.94	2.18	1.04	1.15	-0.28	4.73	0.02
$BaPbO_3$	-15.41	9.84	3.92	5.92	-0.82	4.79	0.00
$YGaO_3$	-13.11	9.87	3.94	5.92	-0.95	4.89	0.00
$KOsO_3$	-2.29	6.02	1.71	4.32	-2.96	4.69	1.45
$LaPdO_3$	-2.07	8.46	2.77	5.69	-1.52	4.72	1.18
$YTlO_3$	-10.83	9.84	3.92	5.91	-1.97	4.77	0.01
$ScTlO_3$	-10.32	9.84	3.93	5.90	-0.62	4.82	0.02
$SrMoO_3$	-1.20	4.47	1.29	3.18	-3.57	4.79	1.41
$BaTeO_3$	-38.32	9.87	3.95	5.92	-1.58	4.91	0.00
$YPdO_3$	-2.04	8.50	2.75	5.75	-1.73	4.73	0.86
$LaTaO_3$	-0.30	3.40	1.06	2.34	-4.97	4.75	1.40
$CaSnO_3$	-21.12	9.87	3.95	5.92	-1.52	4.97	0.00
$SrScO_3$	4.69	1.56	0.83	0.73	-0.45	4.88	0.06

Continued on next page

Formula	d-center (eV)	d-filling	e_g-filling	t_{2g}-filling	p-center (eV)	p-filling	d-states at E_f
$NaLaO_3$	5.38	1.83	0.91	0.92	-0.94	4.70	0.05
$NaMoO_3$	-1.24	4.29	1.43	2.86	-3.09	4.69	1.19
$ScIrO_3$	-2.04	7.25	2.48	4.78	-3.23	4.77	0.76
$LaCoO_3$	-1.26	7.26	2.05	5.20	-1.80	4.70	4.69
KYO_3	5.87	1.51	0.77	0.74	-0.06	4.62	0.09
$SrReO_3$	-1.91	5.28	1.38	3.90	-3.91	4.81	1.64
$LaAuO_3$	-3.25	9.10	3.26	5.84	-1.83	4.72	0.46
$LaReO_3$	-1.45	5.42	1.48	3.94	-4.45	4.71	1.26
$KRhO_3$	-2.28	7.15	2.23	4.91	-1.69	4.57	2.39
$SrPbO_3$	-15.49	9.84	3.93	5.92	-1.18	4.92	0.00
$NaTeO_3$	-38.00	9.87	3.95	5.92	-1.41	4.95	0.00
$CaVO_3$	-0.65	3.41	1.24	2.17	-2.96	4.71	1.71
$ScBiO_3$	-23.64	9.87	3.95	5.92	-3.49	4.94	0.00
$YZnO_3$	-5.42	9.75	3.83	5.92	-1.35	4.93	0.14
$CaBiO_3$	-22.05	9.87	3.95	5.92	-1.19	4.94	0.00
$BaZrO_3$	2.52	2.18	1.07	1.12	-1.35	4.81	0.00
$YScO_3$	4.09	1.61	0.91	0.71	-1.27	4.88	0.00
$SrAuO_3$	-2.95	8.97	3.19	5.79	-1.02	4.76	0.43
$KSnO_3$	-20.49	9.88	3.95	5.92	-0.57	4.87	0.00
$NaVO_3$	-0.47	3.37	1.45	1.93	-2.23	4.57	0.09
$CaCoO_3$	-1.66	7.18	2.16	5.02	-1.48	4.59	3.84
$NaOsO_3$	-2.41	5.99	1.70	4.29	-3.11	4.68	1.33
$SrRuO_3$	-1.97	6.44	1.86	4.58	-2.17	4.69	2.76
$YNbO_3$	-0.61	3.60	1.10	2.50	-4.97	4.75	1.52
$YIrO_3$	-1.43	7.34	2.23	5.11	-3.03	4.71	3.74
$ScHgO_3$	-5.74	9.77	3.88	5.89	-2.11	4.80	0.18
$YBiO_3$	-23.74	9.87	3.95	5.92	-3.19	4.90	0.00
$CaRhO_3$	-2.00	7.24	2.22	5.02	-2.13	4.68	3.37
$YCdO_3$	-6.87	9.76	3.86	5.90	-1.35	4.80	0.15
$YGeO_3$	-25.28	9.87	3.95	5.92	-2.96	4.86	0.00
$SrTlO_3$	-10.12	9.80	3.89	5.92	-0.84	4.86	0.06
$CaOsO_3$	-2.15	6.08	2.03	4.05	-2.80	4.68	1.12
$SrZrO_3$	2.53	2.27	1.08	1.19	-1.54	4.93	0.00
$ScInO_3$	-13.85	9.85	3.93	5.92	-2.77	4.91	0.00
$BaVO_3$	-0.54	3.34	1.22	2.12	-2.41	4.67	1.66
$CaPdO_3$	-2.21	8.33	2.81	5.52	-1.22	4.67	2.37
$YCaO_3$	6.24	0.99	0.52	0.46	-0.78	4.81	0.13
$BaCoO_3$	-1.48	7.21	2.22	4.99	-1.19	4.57	3.94
$SrPdO_3$	-2.27	8.33	2.93	5.40	-1.29	4.69	2.29
$LaGeO_3$	-24.71	9.87	3.95	5.92	-2.25	4.86	0.00
$YBaO_3$	3.34	1.10	0.46	0.64	-2.61	4.82	0.04

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Formula	d-center (eV)	d-filling	e_g-filling	t_{2g}-filling	p-center (eV)	p-filling	d-states at E_f
$SrVO_3$	-0.63	3.40	1.24	2.17	-2.77	4.78	1.64
$LaZrO_3$	0.08	2.37	1.03	1.34	-4.75	4.80	1.28
$BaAuO_3$	-2.96	9.00	3.22	5.77	-0.85	4.62	0.55
$YSbO_3$	-30.69	9.87	3.95	5.92	-4.00	4.90	0.00
$LaSnO_3$	-20.67	9.87	3.95	5.92	-1.72	4.86	0.00
$LaBiO_3$	-23.31	9.87	3.95	5.92	-2.63	4.92	0.00
$ScVO_3$	-0.73	3.59	1.13	2.46	-4.71	4.75	2.37
$NaSbO_3$	-29.61	9.87	3.95	5.92	-2.04	5.01	0.00
$CaReO_3$	-1.98	5.28	1.37	3.90	-4.28	4.76	1.67
$CaBaO_3$	5.11	1.30	0.51	0.79	-0.41	4.82	0.09
$SrNiO_3$	-1.74	8.09	2.63	5.46	-1.15	4.63	3.15
$BaBaO_3$	5.20	1.21	0.49	0.73	-0.33	4.76	0.07
$SrIrO_3$	-1.85	7.21	2.58	4.64	-2.50	4.73	1.84
$BaPdO_3$	-2.20	8.37	2.95	5.42	-1.08	4.59	2.19
$SrSbO_3$	-29.00	9.87	3.95	5.92	-1.88	5.07	0.00
$BaNiO_3$	-1.68	8.12	2.69	5.43	-0.97	4.55	2.97
$ScNbO_3$	-0.83	3.60	1.16	2.44	-5.18	4.80	1.59
$CaCuO_3$	-2.42	9.13	3.28	5.86	-0.90	4.61	0.41
$KIrO_3$	-2.51	6.98	2.16	4.81	-2.18	4.61	2.21
$BaScO_3$	4.66	1.49	0.81	0.68	-0.23	4.74	0.08
$YMgO_3$	5.81	0.49	0.20	0.29	-0.61	4.83	0.03
$YLaO_3$	3.59	1.76	0.92	0.84	-2.13	4.82	0.00
$YSnO_3$	-20.57	9.87	3.95	5.92	-1.62	4.85	0.00
$ScZrO_3$	0.52	2.55	1.04	1.51	-4.86	4.84	0.28
$LaHgO_3$	-5.73	9.67	3.77	5.90	-1.62	4.77	0.18
$SrAgO_3$	-3.22	9.21	3.36	5.85	-0.80	4.72	0.29
$LaMoO_3$	-1.24	4.58	1.32	3.26	-4.82	4.68	1.38
$LaMgO_3$	6.10	0.52	0.22	0.30	-0.52	4.80	0.03
YYO_3	4.28	1.67	0.89	0.78	-1.69	4.82	0.00
$KBiO_3$	-22.07	9.87	3.95	5.92	-0.85	4.88	0.00
$ScCoO_3$	-1.26	7.29	1.86	5.43	-2.69	4.76	3.80
$KCuO_3$	-2.55	9.10	3.31	5.80	-0.63	4.48	0.88
$NaHfO_3$	4.67	2.13	1.01	1.12	-0.19	4.69	0.02
$CaTiO_3$	1.71	2.02	1.02	1.00	-1.90	4.96	0.00
$SrGeO_3$	-24.82	9.87	3.95	5.92	-1.25	4.96	0.00
$ScZnO_3$	-5.56	9.76	3.85	5.92	-2.18	5.02	0.15
$NaGeO_3$	-24.32	9.87	3.95	5.92	-0.78	4.80	0.00
$BaGeO_3$	-24.73	9.87	3.95	5.92	-0.87	4.82	0.00
$SrSnO_3$	-20.94	9.87	3.95	5.92	-1.23	5.03	0.00
$YPtO_3$	-1.77	8.29	2.60	5.69	-2.31	4.73	0.79
$SrNbO_3$	-0.70	3.46	1.18	2.28	-3.94	4.86	1.35

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Formula	d-center (eV)	d-filling	e_g-filling	t_{2g}-filling	p-center (eV)	p-filling	d-states at E_f
$BaGaO_3$	-13.00	9.87	3.94	5.92	-0.35	4.72	0.01
$CaGaO_3$	-12.77	9.87	3.94	5.92	-0.53	4.81	0.01
$ScOsO_3$	-1.58	6.47	1.85	4.62	-3.65	4.78	1.62
$KZnO_3$	-4.86	9.75	3.83	5.91	-0.82	4.74	0.18
$KAgO_3$	-3.14	9.21	3.39	5.82	-0.66	4.55	0.61
$CaPbO_3$	-15.66	9.84	3.93	5.92	-1.46	4.85	0.00
$SrRhO_3$	-2.10	7.21	2.25	4.96	-2.00	4.69	3.04
$NaTiO_3$	2.99	2.00	0.99	1.01	-0.79	4.79	0.03
$BaPtO_3$	-1.94	8.10	2.81	5.28	-1.51	4.65	2.20
$BaNbO_3$	-0.57	3.36	1.17	2.19	-3.59	4.76	1.37
YVO_3	-0.59	3.51	1.04	2.46	-4.20	4.73	2.19
$ScGaO_3$	-13.82	9.86	3.94	5.92	-2.19	4.92	0.00
$ScCrO_3$	-1.21	4.61	1.22	3.39	-4.53	4.75	2.94
$SrBiO_3$	-22.24	9.87	3.95	5.92	-1.33	5.03	0.00
$LaFeO_3$	-1.09	6.38	1.55	4.83	-2.19	4.69	4.63
$KHgO_3$	-5.24	9.56	3.67	5.89	-0.63	4.60	0.20
$BaCuO_3$	-2.33	9.14	3.31	5.83	-0.65	4.54	0.89
$KTeO_3$	-38.12	9.87	3.95	5.92	-1.37	4.94	0.00
$SrPtO_3$	-1.97	8.07	2.77	5.30	-1.69	4.77	2.32
$KPtO_3$	-2.42	8.01	2.86	5.15	-1.66	4.61	1.70
$ScRuO_3$	-1.53	6.57	2.09	4.47	-2.53	4.63	2.47
$CaLaO_3$	4.35	1.76	0.88	0.89	-0.94	4.82	0.14
$CaCdO_3$	-6.61	9.69	3.79	5.91	-0.70	4.76	0.12
$NaCuO_3$	-2.54	9.10	3.29	5.81	-0.76	4.50	0.95
$LaWO_3$	-0.51	4.34	1.37	2.97	-3.76	4.76	0.59
$SrGaO_3$	-12.86	9.87	3.94	5.92	-0.49	4.84	0.01
$BaYO_3$	5.18	1.55	0.81	0.74	-0.29	4.74	0.07
$KSbO_3$	-29.38	9.79	3.87	5.92	-1.68	5.01	0.00
$LaPbO_3$	-15.46	9.86	3.94	5.91	-1.03	4.84	0.00
$YNiO_3$	-1.33	8.18	2.53	5.66	-1.53	4.71	2.32
$LaAgO_3$	-3.47	9.26	3.39	5.87	-1.33	4.71	0.35
$SrTeO_3$	-38.50	9.87	3.95	5.92	-2.04	5.08	0.00
$SrYO_3$	5.21	1.64	0.83	0.81	-0.40	4.83	0.07
$LaRuO_3$	-1.44	6.61	1.67	4.93	-2.64	4.72	3.58
$CaMoO_3$	-0.57	4.37	1.64	2.73	-3.21	4.73	2.00
$LaCdO_3$	-6.75	9.74	3.84	5.91	-1.05	4.79	0.14
$CaYO_3$	5.00	1.64	0.84	0.80	-0.54	4.82	0.05
$NaCdO_3$	-6.34	9.69	3.78	5.91	-0.44	4.61	0.14
$YCoO_3$	-1.24	7.24	1.94	5.30	-2.01	4.71	4.42
$CaTeO_3$	-38.89	9.87	3.95	5.92	-2.60	4.98	0.00
$LaTlO_3$	-10.62	9.83	3.92	5.91	-1.65	4.80	0.01

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Formula	d-center (eV)	d-filling	e_g-filling	t_{2g}-filling	p-center (eV)	p-filling	d-states at E_f
$YHfO_3$	0.25	2.28	1.05	1.24	-5.15	4.79	0.64
$BaBiO_3$	-22.22	9.87	3.95	5.92	-1.13	4.88	0.00
$CaZrO_3$	2.27	2.25	1.10	1.15	-1.97	4.85	0.00
$KScO_3$	4.78	1.49	0.78	0.71	-0.34	4.70	0.09
$BaHfO_3$	2.79	2.14	1.03	1.11	-1.45	4.82	0.00
$YOsO_3$	-1.47	6.42	2.37	4.04	-3.64	4.72	1.24
$LaNiO_3$	-1.37	8.20	2.63	5.58	-1.32	4.70	2.66
$NaAuO_3$	-2.99	8.93	3.19	5.73	-0.86	4.59	0.65
$YTiO_3$	0.36	2.22	0.85	1.37	-4.70	4.91	1.57
$LaYO_3$	4.49	1.63	0.87	0.77	-1.23	4.83	0.00
$SrHfO_3$	2.96	2.24	1.05	1.19	-1.46	4.92	0.00
$BaLaO_3$	4.51	1.70	0.88	0.83	-0.72	4.74	0.12
$KReO_3$	-1.82	5.07	1.48	3.60	-3.43	4.72	1.41
$LaCuO_3$	-2.40	9.17	3.29	5.88	-0.95	4.69	0.54
$KPdO_3$	-2.81	8.21	2.74	5.46	-1.00	4.51	1.86
$LaCaO_3$	6.39	0.97	0.52	0.45	-0.57	4.80	0.14
$NaZnO_3$	-5.04	9.72	3.81	5.91	-0.88	4.74	0.16
$KTaO_3$	-0.41	2.93	1.23	1.70	-3.52	4.80	0.46
$LaSbO_3$	-30.17	9.87	3.95	5.92	-3.34	4.92	0.00
$CaNbO_3$	-0.68	3.47	1.18	2.30	-4.21	4.80	1.33
$CaNiO_3$	-1.61	8.12	2.73	5.40	-1.29	4.62	3.13
$CaAuO_3$	-3.04	8.98	3.17	5.81	-1.09	4.71	0.18
$CaPtO_3$	-1.88	8.10	2.73	5.37	-1.71	4.73	2.21
$SrHgO_3$	-5.47	9.56	3.66	5.89	-0.92	4.80	0.16
$YRhO_3$	-1.76	7.40	2.08	5.32	-2.10	4.74	1.24
$ScNiO_3$	-1.35	8.25	2.50	5.75	-2.20	4.76	1.42
$YAgO_3$	-3.57	9.28	3.41	5.86	-1.65	4.72	0.38
$BaTiO_3$	1.59	1.98	0.98	0.99	-1.53	4.89	0.00
$NaWO_3$	-1.06	4.04	1.32	2.72	-3.74	4.75	1.12
$BaTaO_3$	-0.41	3.20	1.12	2.08	-4.16	4.76	1.32
$SrZnO_3$	-5.08	9.74	3.82	5.92	-1.03	4.91	0.14
$CaScO_3$	4.72	1.57	0.85	0.72	-0.41	4.85	0.05
$LaCrO_3$	-1.04	4.52	1.13	3.40	-3.45	4.73	3.09
$YRuO_3$	-1.40	6.63	1.65	4.98	-2.83	4.72	3.43
$NaCrO_3$	-1.27	4.39	1.55	2.84	-2.20	4.60	1.40
$CaHgO_3$	-5.63	9.55	3.66	5.89	-1.09	4.75	0.16
$YMoO_3$	-1.26	4.69	1.20	3.49	-4.72	4.73	1.76
$LaTiO_3$	0.36	2.16	0.84	1.32	-4.26	4.92	1.56
$ScCaO_3$	6.19	0.87	0.40	0.47	-0.43	4.88	0.02
$LaLaO_3$	3.90	1.73	0.90	0.83	-1.62	4.84	0.00
$CaRuO_3$	-2.01	6.43	1.81	4.62	-2.40	4.68	3.07

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Formula	d-center (eV)	d-filling	e_g-filling	t_{2g}-filling	p-center (eV)	p-filling	d-states at E_f
$LaBaO_3$	3.56	1.11	0.47	0.64	-2.25	4.84	0.04
$LaGaO_3$	-13.01	9.86	3.94	5.92	-0.63	4.87	0.00
$KGeO_3$	-24.36	9.87	3.95	5.92	-0.72	4.79	0.00
$KLaO_3$	5.28	1.73	0.87	0.87	-0.62	4.66	0.08
$LaZnO_3$	-5.29	9.75	3.83	5.92	-1.03	4.92	0.13
$LaNbO_3$	-0.56	3.58	1.08	2.50	-4.66	4.76	1.52
$CaHfO_3$	2.62	2.22	1.06	1.16	-1.95	4.85	0.00
$KHfO_3$	4.43	2.15	1.01	1.14	-0.25	4.73	0.02
$SrLaO_3$	4.42	1.79	0.89	0.91	-0.90	4.88	0.14
$SrInO_3$	-12.49	9.84	3.92	5.92	-0.68	4.93	0.05
$BaIrO_3$	-1.77	7.16	2.58	4.57	-2.26	4.62	1.84
$ScRhO_3$	-1.97	7.35	2.34	5.01	-2.71	4.78	1.38
$NaHgO_3$	-5.40	9.54	3.65	5.89	-0.67	4.63	0.18
$KNbO_3$	-0.43	3.13	1.30	1.83	-2.82	4.77	0.36
$NaZrO_3$	4.17	2.17	1.04	1.13	-0.23	4.69	0.02
$LaIrO_3$	-1.43	7.34	2.28	5.06	-2.80	4.71	3.67
$CaWO_3$	-1.00	4.20	1.20	3.00	-4.42	4.77	1.29
$LaTeO_3$	-38.33	9.87	3.95	5.92	-3.56	4.81	0.00
KWO_3	-1.07	4.03	1.32	2.72	-3.61	4.76	1.14
$SrCdO_3$	-6.49	9.70	3.80	5.91	-0.68	4.80	0.12
$ScAgO_3$	-3.70	9.34	3.48	5.86	-2.33	4.76	0.39
$NaTaO_3$	-0.38	2.92	1.24	1.68	-3.60	4.77	0.39
$BaReO_3$	-1.78	5.22	1.37	3.85	-3.62	4.71	1.69
$KCdO_3$	-6.23	9.72	3.80	5.91	-0.44	4.60	0.15
$ScScO_3$	3.29	1.70	0.94	0.77	-2.65	4.91	0.00
$LaOsO_3$	-1.40	6.43	2.25	4.17	-3.76	4.72	2.08
$ScYO_3$	3.52	1.75	0.91	0.84	-2.77	4.83	0.01
$CaSbO_3$	-28.83	9.87	3.95	5.92	-1.71	4.96	0.00
$NaNbO_3$	-0.45	3.11	1.30	1.81	-2.93	4.75	0.34
$LaHfO_3$	0.19	2.23	1.04	1.19	-4.90	4.80	0.86
$CaIrO_3$	-1.85	7.21	2.55	4.67	-2.67	4.71	2.06
$LaRhO_3$	-1.54	7.41	2.07	5.34	-2.24	4.71	2.39
$ScPdO_3$	-2.62	8.40	2.89	5.51	-2.45	4.76	1.21
$YPbO_3$	-15.52	9.86	3.95	5.91	-1.15	4.83	0.00
$KMnO_3$	-1.19	5.11	1.69	3.42	-1.71	4.53	3.18
$NaSnO_3$	-20.38	9.87	3.95	5.92	-0.51	4.83	0.00
$SrTaO_3$	-0.49	3.26	1.14	2.12	-4.43	4.87	1.27
$KMoO_3$	-1.23	4.28	1.43	2.86	-2.99	4.70	1.22
$KTiO_3$	2.85	2.00	0.98	1.02	-0.83	4.82	0.03
YWO_3	-0.29	4.46	1.66	2.80	-4.08	4.73	1.16
$KNiO_3$	-1.91	8.08	2.63	5.46	-0.91	4.50	2.03

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Formula	d-center (eV)	d-filling	e_g-filling	t_{2g}-filling	p-center (eV)	p-filling	d-states at E_f
$CaGeO_3$	-24.93	9.87	3.95	5.92	-1.40	4.92	0.00
$NaPbO_3$	-15.07	9.84	3.92	5.92	-0.55	4.75	0.01
$YAuO_3$	-3.40	9.12	3.28	5.84	-2.20	4.72	0.46
$KPbO_3$	-15.12	9.85	3.92	5.92	-0.56	4.76	0.01
$BaRhO_3$	-2.01	7.22	2.25	4.97	-1.81	4.61	3.07
$YTaO_3$	-0.34	3.40	1.08	2.32	-5.24	4.75	1.38
$YTeO_3$	-38.45	9.87	3.95	5.92	-3.84	4.79	0.00
$ScCuO_3$	-2.72	9.20	3.33	5.88	-2.10	4.74	0.51
$BaHgO_3$	-5.38	9.57	3.67	5.90	-0.66	4.66	0.17
$NaBiO_3$	-22.08	9.87	3.95	5.92	-0.94	4.88	0.00
$CaTlO_3$	-10.22	9.81	3.89	5.91	-0.98	4.80	0.07
$BaInO_3$	-12.49	9.84	3.92	5.92	-0.46	4.78	0.05
$BaTlO_3$	-10.05	9.81	3.89	5.92	-0.57	4.72	0.06
$BaMnO_3$	-0.97	5.13	1.46	3.67	-1.92	4.56	3.31
$BaSbO_3$	-29.17	9.87	3.95	5.92	-1.71	4.90	0.00
$SrBaO_3$	5.16	1.32	0.52	0.80	-0.54	4.97	0.12
$YZrO_3$	0.20	2.44	1.03	1.41	-4.98	4.79	1.04
$ScTiO_3$	0.35	2.26	0.91	1.35	-5.08	4.95	0.92
$BaSnO_3$	-20.91	9.87	3.95	5.92	-0.96	4.90	0.00
$LaScO_3$	4.32	1.57	0.88	0.70	-0.76	4.89	0.01
$KRuO_3$	-2.00	6.34	1.94	4.40	-1.84	4.56	2.06
$KAuO_3$	-2.93	8.97	3.24	5.72	-0.85	4.59	0.71
$CaAgO_3$	-3.32	9.20	3.35	5.85	-0.80	4.69	0.18
$LaInO_3$	-12.89	9.84	3.93	5.92	-1.22	4.89	0.01

6 Distortion effects in 2x2 cubic unit cells

To comment on the effects of local octahedral distortion, we include additional data here on a subset of the data calculated in the ideal cubic phase. These distortions may occur as the result of Jahn-Teller symmetry breaking or simply if strained octahedra fill the unit cell more optimally than cubically aligned ones (as described by the Goldschmidt tolerance factor).

Perturbations to adsorption energies are generally small, with a median value of 0.1 eV, but also are systematic (i.e. nearly all positive). This suggests that local distortion during ionic relaxation may cause oxygenates to adsorb more weakly. We speculate that partial quenching of structural frustration via these allowed distortions in the unadsorbed state leads to a less exergonic adsorption bond. We also note that, while the perturbations are not trivial in every individual case, the trends we focus on in the main text are preserved between the distorted and cubic phases. Detailed studies of individual compounds, however, may require more careful treatment of the ground-state crystal structure.

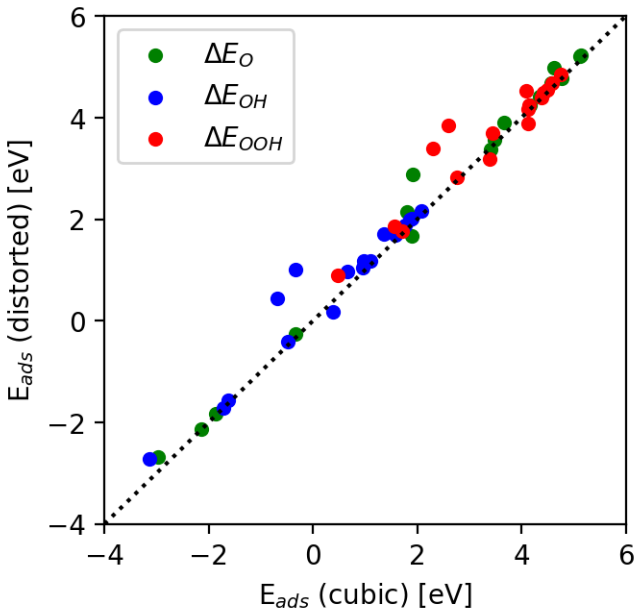

Figure 1: Plot of the adsorption energies of surfaces derived from structures with (y-axis) and without (x-axis) allowed distortions of the 2x2 crystal structure. Plot shows data for adsorption of OOH* (red), OH* (blue) and O* (green).

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