SUPPLEMENTARY INFORMATION

Overcoming Hurdles in Oxygen Evolution Catalyst Discovery via Co-Design

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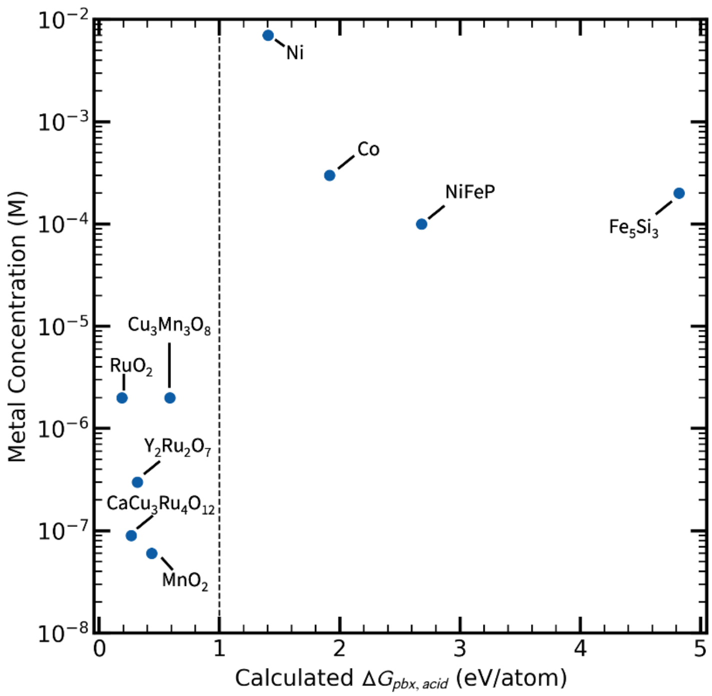

Figure S1: Establishment of as a reasonable upper limit of $\Delta G_{pbx}$for operationally-stable catalysts for OER in acid. Using catalysts from Figure 4, the experimentally measured dissolved metal concentrations are shown as a function of the calculated $\Delta G_{pbx,acid}$(pH=1). Only materials with a known computational bulk structure are shown. Metal concentrations below 10^{-5} M are observed only for materials below the ΔG_{pbx} threshold of 1eV/metal atom (vertical dashed line).

Table S1: List of d_0 descriptors for each of the transition metal elements considered in this study.

	Acid (pH= 1)		Alkaline (pH=14)	
Element	d_0	End Member	d_0	End Member
Sc	0	$Sc^{+3}_{(aq)}$	0	Sc_2O_3
Ti	0	TiO_2	0	TiO_2
V	0	$VO_4^-{}_{(aq)}$	0	$VO_4^-{}_{(aq)}$
Cr	0	$CrHO_4^-$	0	CrO_4^{2-}
Mn	3	MnO_2	0	MnO_4^-
Fe	4	$Fe^{+3}_{(aq)}$	4	Fe_2O_3
Co	7	$Co^{+2}_{(aq)}$	6	CoOOH , $Li(CoO_2)_2$, $LaCoO_3$
Ni	8	$Ni^{+2}_{(aq)}$	8	$Ni(OH)_3^-{}_{(aq)}$, $LaNiO_3$
Cu	9	$Cu^{+2}_{(aq)}$	8	Cu_2O_3, $LaCuO_3$, $Zn(CuO_2)_2$, $Ca(CuO_2)_2$
Zn	10	$Zn^{+2}_{(aq)}$	10	$ZnO_2^{-2}{}_{(aq)}$, $Zn(CuO_2)_2$
Y	0	$Y^{+3}_{(aq)}$	0	Y_2O_3
Zr	0	$ZrO^{+2}_{(aq)}$	0	ZrO_2
Nb	0	$Nb(HO)_{5\,(aq)}$	0	$NbO_3^-{}_{(aq)}$
Mo	0	MoO_3	0	$MoO_4^{-2}{}_{(aq)}$
Tc	0	Tc_2O_7	0	$TcO_4^-{}_{(aq)}$
Ru	0	RuO_4	0	RuO_4
Rh	5	RhO_2	5	RhO_2
Pd	6	PdO_2	6	PdO_2
Ag	10	$Ag^{+}_{(aq)}$	9	AgO
Cd	10	$Cd^{+2}_{(aq)}$	10	$Cd(OH)_{2\,(aq)}$
Hf	0	$Hf^{+4}_{(aq)}$	0	HfO_2
Ta	2	$TaO_2^+{}_{(aq)}$	0	Ta_2O_5 , $SrTa_2O_6$

W	0	WO_3	0	$WO_4^{-2}{}_{(aq)}$
Re	0	$ReO_4^{-}{}_{(aq)}$	0	$ReO_4^{-}{}_{(aq)}$
Os	0	OsO_4	0	OsO_4
Ir	2	$IrO_4^{-}{}_{(aq)}$	2	$IrO_4^{-}{}_{(aq)}$
Pt	6	PtO_2 / $BiPt_3O_{11}$	6	$BiPt_3O_{11}$, $La_3Pt_3O_{11}$, PtO_2
Au	9	$H_3AuO_{3\ (aq)}$	9	$H_2AuO_3^{-}{}_{(aq)}$, Bi_2AuO_5, $Sr(AuO_2)_2$, $LaAuO_3$

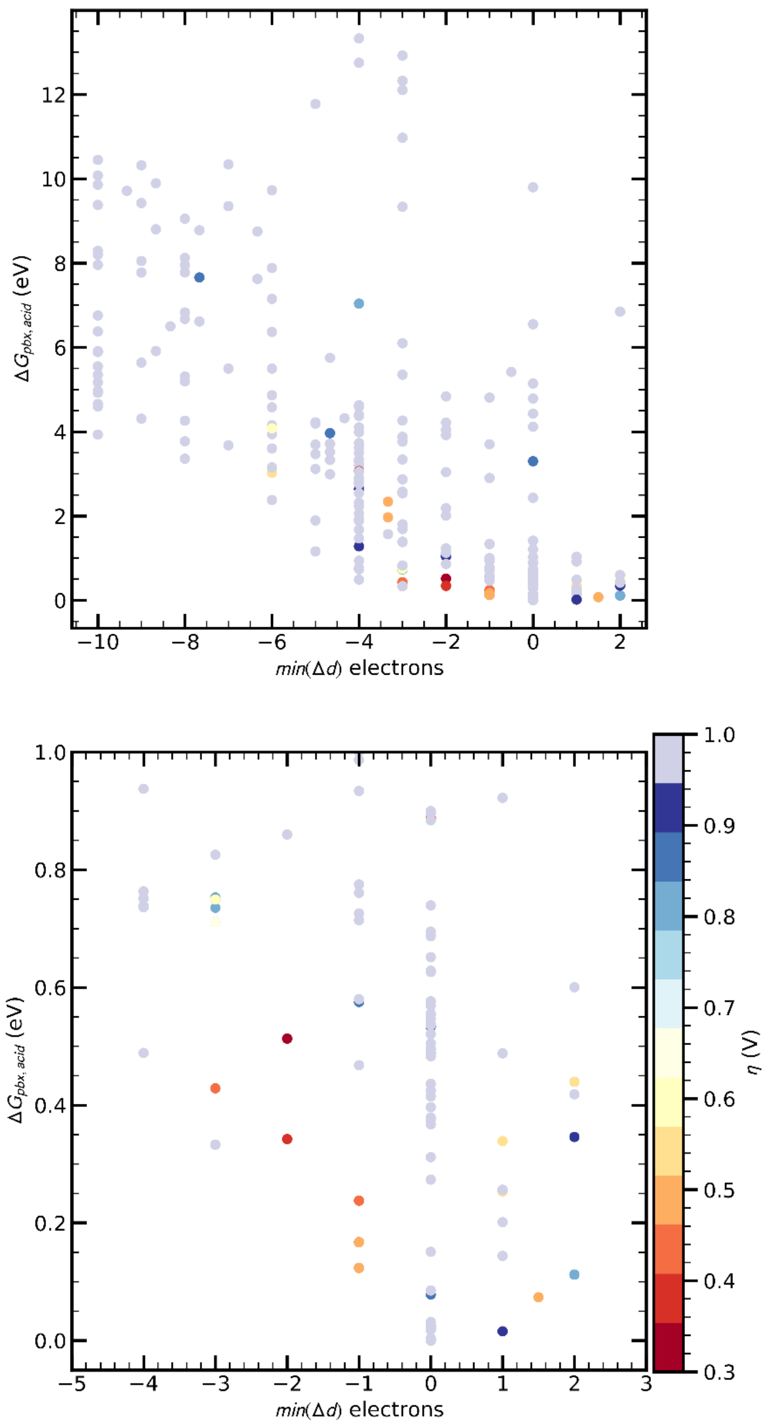

Figure S2: The analogue of Figure 6 using an alternative acid stability descriptor, the minimum Δd among all cations in the catalyst. The bottom panel has a maximum ΔG_{pbx} of 1 eV/atom, for which all considered materials have $min(\Delta d)$ no lower than -4 and no greater than 2.