Electronic Supplementary Information (ESI): Optimizing accuracy and efficacy in data-driven materials discovery for the solar production of hydrogen

Y. Xiong,[a] Q. T. Campbell,[b] J. Fanghanel,[a,c] C. K. Badding,[d] H. Wang,[a] N. E. Kirchner-Hall,[a] M. J. Theibault,[d] I. Timrov,[e] J. S. Mondschein,[c] K. Seth,[c] R. R. Katzbaer,[c] A. Molina Villarino,[d] B. Pamuk,[f] M. E. Penrod,[a] M. M. Khan,[a] T. Rivera,[c] C. Smith,[g] X. Quintana,[a] P. Orbe,[a] C. J. Fennie,[f] S. Asem-Hiablie,[h] J. L. Young,[i] T. G. Deutsch,[i] M. Cococcioni,[j] V. Gopalan,[a] H. D. Abruña,[d] R. E. Schaak,[c] I. Dabo[a]

[a] *Department of Materials Science and Engineering, and Materials Research Institute, The Pennsylvania State University, University Park, PA, USA*
[b] *Sandia National Laboratories, Albuquerque, NM, USA*
[c] *Department of Chemistry and Materials Research Institute, The Pennsylvania State University, University Park, PA, USA*
[d] *Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, USA*
[e] *Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*
[f] *School of Applied and Engineering Physics, Cornell University, Ithaca, NY, USA*
[g] *Department of Materials Science and Engineering, Northwestern University, Evanston, IL, USA*
[h] *Department of Agricultural and Biological Engineering, The Pennsylvania State University, University Park, PA, USA*
[i] *National Renewable Energy Laboratory, Golden, CO, USA*
[j] *Department of Physics, University of Pavia, Pavia, Italy*

S1. Criteria of the literature survey

The literature survey was performed using the Web of Science database by applying the criteria in Fig. S1. The initial search returned 626 publications, which were then examined individually. Publications focusing exclusively on experimental synthesis and/or characterization were removed from the literature survey. Computational studies with less than 50 candidate materials were also not considered. Using this approach, we identified 202 papers. These articles were read to categorize them into technological areas and determine whether they include validation experiments. The results of the survey are shown in Fig. 1 of the main text.

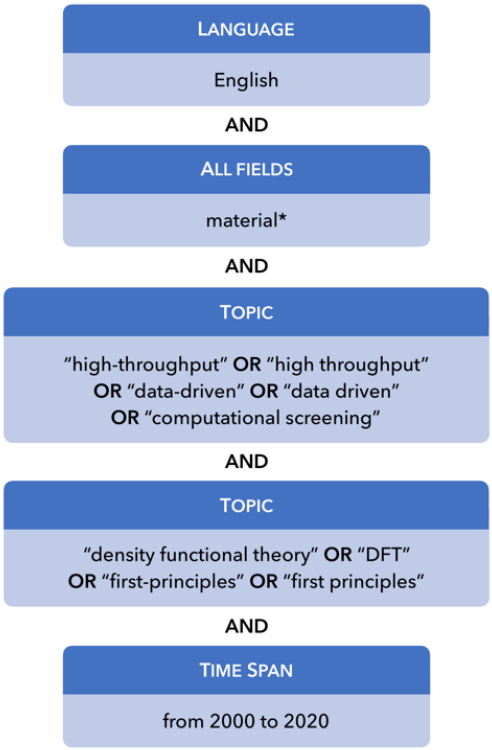


Figure S1 Criteria for the survey of peer-reviewed publications in high-throughput computational materials science.

S2. Criteria of the computational screening

Figure S2 shows the domains spanned by the candidate materials with the Hubbard U correction (Domain A) and without this correction (Domain B). Domain A is delimited by the standard criteria of water splitting: $1.5 < \varepsilon_g < 2.5$ eV, $E_{VB} > 1.2$ V vs. SHE, and $E_{CB} < 0$ V vs. SHE, as discussed in the main text. Domain B is constructed by rescaling the band gap $\varepsilon_g = e(E_{VB} - E_{CB})$ of each point in Domain A by a factor γ while keeping the flatband potential $E_{FB} = (E_{VB} + E_{CB})/2$ constant. Explicitly, the γ-dependent transformation T_γ can be written as $(E_{VB}, E_{CB}) \rightarrow (E_{VB} - (1 - \gamma)\ (E_{VB} - E_{CB})/2,\ E_{CB} + (1 - \gamma)\ (E_{VB} - E_{CB})/2)$. Domain B is obtained by merging all the images of Domain A through T_γ for γ ranging from 0.5 to 0.8 (corresponding to the typical margin of error of band gaps within DFT). The resulting criteria are $0.75 < \varepsilon_g < 2$ eV, $E_{VB} > 0.575$ V vs. SHE, and $E_{CB} < 0.625$ V vs. SHE. These criteria are used in the screening outlined in Fig. 2 of the main text.

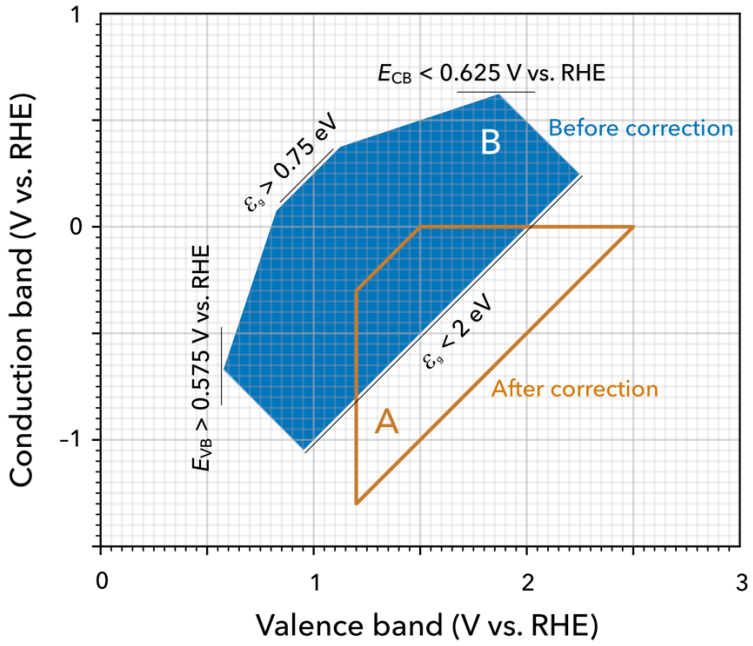


Figure S2 Domains spanned by admissible candidates with Hubbard U correction (Domain A, orange) and without correction (Domain B, blue).

S3. Calculations of band gap and band edges

The band gaps and band edges computed using DFT and DFT+U are reported in Table S1. The distributions of the U parameters calculated from first principles using linear-response theory are provided in Fig. S3. For comparison, we summarized the band gaps from the Materials Project in Table S2.

Table S1 Band gaps and band edges of the 162 candidate photocatalysts calculated using DFT with the PBE functional and DFT+*U*. The *U* parameters are computed from first principles *via* one-shot calculations within density-functional perturbation theory (DFPT)[1] using the QUANTUM ESPRESSO distribution.[2,3] "None" indicates that the compound does not contain elements on which the Hubbard correction is applied. Orthogonalized atomic orbitals are selected as projectors on the Hubbard manifold using the Löwdin method. The structures are optimized at the DFT level (*i.e.* without the Hubbard *U* correction). To enable systematic sorting, the elements in the chemical formula are ordered by increasing electronegativity, following the naming convention of the Materials Project (the conventional nomenclature is used in the main text). The space group and the *U* parameters are provided for each compound. Band edges are reported relative to the reversible hydrogen electrode (RHE). The absolute value of the hydrogen electrode potential is of 4.44 V. Calculations that could not go through the computational cycle are marked as "DFT incomplete", "DFPT incomplete" and "DFT+*U* incomplete" to indicate of an incomplete convergence in computing the DFT ground state, the Hubbard *U* parameters, and the DFT+*U* ground state, respectively. DFT and DFT+*U* data are reported for two $CaIn_2O_4$ phases (the cubic phase and the experimentally observed orthorhombic phase).

	Space group	U parameters (eV)	DFT ε_g (eV)	DFT eE_{CB} (eV)	DFT eE_{VB} (eV)	DFT+U ε_g (eV)	DFT+U eE_{CB} (eV)	DFT+U eE_{VB} (eV)
$AlCuO_2$	$R\bar{3}m$	10.3 (Cu-3*d*), 9.2 (O-2*p*)	1.78	0.02	1.81	3.07	–0.62	2.45
$Ba_2Fe_2O_5$	$P2_1/c$	×	DFT incomplete			×	×	×
$Ba_2In_2S_5$	$Pbca$	None	2.04	–1.15	0.89	—	—	—
Ba_2PbO_4	$I4/mmm$	8.9 (O-2*p*)	1.30	–0.14	1.16	2.05	–0.51	1.53
$Ba_2SnSe_3F_2$	$Pnma$	None	1.72	–0.08	1.64	—	—	—
$Ba_3MnNb_2O_9$	$P\bar{3}m1$	8.1 (Mn-3*d*), 3.3 (Nb-4*d*), 8.4 (O-2*p*)	0.62	0.51	1.13	3.04	–0.70	2.34
$Ba_3Zn_5In_2O_{11}$	$F\bar{4}3m$	×	DFT incomplete			×	×	×
$Ba_6Mn_5O_{16}$	$Cmce$	5.2 (Mn-3*d*), 8.9 (O-2*p*)	0.75	0.31	1.07	0.78	0.30	1.08
$Ba_6V_4S_{11}O_5$	$Pnma$	×	DFT incomplete			×	×	×
$Ba_8Sb_6S_{17}$	$P2/c$	×	DFT incomplete			×	×	×
$BaAlSi_5N_7O_2$	$P1$	×	3.85	–0.68	3.17	DFPT incomplete		
$BaCaFe_4O_8$	$P\bar{3}1m$	6.4 (Fe-3*d*), 8.4 (O-2*p*)	0.30	0.74	1.04	3.52	–0.87	2.65
$BaCu_2O_2$	$I4_1/amd$	12.7 (Cu-3*d*), 8.2 (O-2*p*)	1.39	–0.27	1.13	3.22	–1.18	2.04
$BaHfN_2$	$P4/nmm$	2.7 (Hf-5*d*), 6.4 (N-2*p*)	1.33	–0.41	0.92	2.12	–0.81	1.32
$BaIn_2O_4$	$P2_1/c$	10.7 (O-2*p*)	1.38	–0.16	1.22	3.09	–1.02	2.07
BaS_2	$C2/c$	None	1.55	–0.69	0.87	—	—	—
$BaSbSe_2F$	$P\bar{1}$	None	1.36	0.19	1.55	—	—	—

[1] Timrov, Marzari, Cococcioni, *Physical Review B* **98**, 085127 (2018).
[2] Giannozzi *et al.*, *Journal of Physics: Condensed Matter* **21**, 395502 (2009).
[3] Giannozzi *et al.*, *Journal of Physics: Condensed Matter* **29**, 465901 (2017).

	Space group	U parameters (eV)	DFT ε_g (eV)	DFT eE_{CB} (eV)	DFT eE_{VB} (eV)	DFT+U ε_g (eV)	DFT+U eE_{CB} (eV)	DFT+U eE_{VB} (eV)
$BaSnS_2$	$P2_1/c$	None	1.74	–0.84	0.90	—	—	—
$Ca_{12}Al_{14}O_{33}$	$C2$	9.7 (O-2p)	2.01	–0.65	1.37	3.73	–1.5	2.23
Ca_2CoO_3	Cm	6.6 (Co-3d), 7.8 (O-2p)	0.00	0.11	0.11	2.70	–1.24	1.46
Ca_2FeClO_3	$P4/nmm$	8.1 (Fe-3d), 8.4 (O-2p)	0.00	0.48	0.48	3.41	–1.22	2.19
Ca_2PbO_4	$Pbam$	8.5 (O-2p)	1.50	–0.36	1.14	2.47	–0.85	1.62
Ca_3PCl_3	$Pm\bar{3}m$	None	1.85	–0.92	0.93	—	—	—
$CaFeClO_2$	$C2/m$	×	DFT incomplete			×	×	×
$CaIn_2O_4$	$Fd\bar{3}m$	8.8 (O-2p)	2.02	–0.55	1.48	4.30	–1.48	2.62
$CaIn_2O_4$	$Pnma$	8.8 (O-2p)	2.03	–0.55	1.48	4.10	–1.58	2.52
$CaSb_{10}S_6O_{10}$	$C2/c$	×	DFT incomplete			×	×	×
$CaTaNO_2$	$Pmc2_1$	3.0 (Ta-5d), 6.4 (N-2p), 8.3 (O-2p)	1.67	–0.09	1.58	2.46	–0.48	1.98
$CoPb_2WO_6$	$C2/m$	6.0 (Co-3d), 3.4 (W-5d), 8.1 (O-2p)	0.00	1.48	1.48	DFT+U incomplete		
Cr_3BO_6	$Pnma$	8.2 (O-2p), 7.5 (Cr-3d)	0.63	1.01	1.64	4.28	–0.81	3.46
$CrPb_5O_8$	$P2_1/c$	×	DFT incomplete			×	×	×
$Cs_4Ta_2S_{11}$	$Pca2_1$	2.7 (Ta-5d)	1.78	–0.70	1.08	1.90	–0.76	1.14
$Cs_4Ti_3S_{14}$	$C2/c$	5.4 (Ti-3d)	1.31	–0.41	0.90	2.16	–0.83	1.32
$Cs_4Zr_3Se_{14}$	$C2/c$	2.6 (Zr-4d)	1.54	–0.66	0.88	1.75	–0.76	0.98
$CsCuO_2$	$Cmcm$	11.3 (Cu-3d), 8.1 (O-2p)	1.04	–0.11	0.94	2.32	–0.74	1.58
$CsGeI_3$	$R3m$	None	1.83	–0.36	1.47	—	—	—
$CsLaNb_2O_7$	$P4/mmm$	×	1.67	0.26	1.93	DFPT incomplete		
$CsMnBr_3$	$P6_3/mmc$	6.3 (Mn-3d)	1.36	0.01	1.37	3.53	–1.08	2.45
$CsMnI_3$	$P6_3/mmc$	6.2 (Mn-3d)	1.02	–0.17	0.85	2.78	–1.05	1.73
$CsSbS_2$	$P2_1/c$	None	1.75	–0.81	0.93	—	—	—
Cu_2WS_4	$P\bar{4}2m$	13.5 (Cu-3d), 3.0 (W-5d)	1.66	0.12	1.78	2.06	–0.08	1.98
Cu_3SbS_3	$P2_12_12_1$	14.8 (Cu-3d)	1.06	0.24	1.31	1.89	–0.17	1.72
$Cu_4Mo_5O_{17}$	$P\bar{1}$	×	DFT incomplete			×	×	×
CuI	$P3m1$	18.0 (Cu-3d)	1.64	0.24	1.88	2.75	–0.31	2.44
CuP_2	$P2_1/c$	14.6 (Cu-3d)	0.86	0.34	1.20	1.02	0.26	1.28
Fe_3BO_6	$Pnma$	5.8 (Fe-3d), 8.6 (O-2p)	0.01	1.47	1.49	3.08	–0.06	3.02
$FeNi_2BO_5$	$Pbam$	×	DFT incomplete			×	×	×

	Space group	U parameters (eV)	DFT ε_g (eV)	DFT eE_{CB} (eV)	DFT eE_{VB} (eV)	DFT+U ε_g (eV)	DFT+U eE_{CB} (eV)	DFT+U eE_{VB} (eV)
Ga_2TeSe_2	$I4_1md$	None	1.65	–0.71	0.93	—	—	—
$GaCuI_4$	$I\bar{4}$	16.7 (Cu-3d)	1.67	0.30	1.97	2.43	–0.08	2.35
$GaCuO_2$	$R\bar{3}m$	10.7 (Cu-3d), 8.1 (O-2p)	0.75	0.53	1.28	2.46	–0.33	2.14
GaN	$P6_3mc$	5.4 (N-2p)	1.72	–0.47	1.25	2.97	–1.09	1.88
GaS	$P6_3/mmc$	None	2.05	–1.00	1.05	—	—	—
Ge_4Se_9	$Pca2_1$	None	1.36	0.34	1.70	—	—	—
GeS	$Pnma$	None	1.24	0.29	1.53	—	—	—
GeSe	$Pnma$	None	0.89	0.32	1.21	—	—	—
$GeSe_2$	$P2_1/c$	None	1.47	0.25	1.72	—	—	—
GeTe	$R3m$	None	0.57	0.30	0.87	—	—	—
In_2O_3	$I2_13$	9.2 (O-2p)	0.95	0.37	1.32	3.59	–0.95	2.64
$In_4Bi_2S_9$	$P2_1/m$	None	1.74	0.07	1.81	—	—	—
InBr	$Cmcm$	None	1.26	–0.22	1.04	—	—	—
InI	$Cmcm$	None	1.33	–0.53	0.80	—	—	—
$InSb_2S_4Br$	$C2/m$	None	1.58	0.26	1.84	—	—	—
$InSb_2S_4Cl$	$C2/m$	None	1.61	0.31	1.92	—	—	—
$InSb_2Se_4Br$	$P\bar{1}$	None	1.15	0.33	1.48	—	—	—
K_2CoCl_4	$Pna2_1$	×	DFT incomplete			×	×	×
K_2NbCuS_4	$Fddd$	1.9 (Nb-4d), 8.8 (Cu-3d)	2.01	–0.98	1.03	2.39	–1.17	1.22
$K_2TaCuSe_4$	$Fddd$	1.7 (Ta-5d), 8.9 (Cu-3d)	1.98	–1.07	0.91	2.28	–1.22	1.06
$K_3LaP_2Se_8$	P_1/c	None	1.72	–0.68	1.04	—	—	—
K_3P_{11}	$Pbcn$	None	1.93	–0.71	1.22	—	—	—
K_3PSe_{16}	Fd–3	None	1.12	0.15	1.26	—	—	—
K_3PSe_4	$Pnma$	None	1.68	–1.09	0.60	—	—	—
$K_3VP_2O_8$	$P2_1$/c	×	0.01	0.93	0.94	DFT incomplete		
$K_4P_{21}I$	$Cmcm$	None	1.30	–0.12	1.18	—	—	—
$KBiP_2Se_6$	$P2_1/c$	None	1.64	0.27	1.91	—	—	—
$KCoO_2$	$I\bar{4}$	6.4 (Co-3d), 8.0 (O-2p)	0.27	0.36	0.63	DFT+U incomplete		
$KCuO_2$	$Cmcm$	11.1 (Cu-3d), 8.1 (O-2p)	0.98	0.05	1.03	2.17	–0.54	1.63
$KLa_5C_2Cl_{10}$	$P2_1/c$	×	DFT incomplete			×	×	×

	Space group	U parameters (eV)	DFT			DFT+U		
			ε_g (eV)	eE_{CB} (eV)	eE_{VB} (eV)	ε_g (eV)	eE_{CB} (eV)	eE_{VB} (eV)
$KNaZnO_2$	$C2/c$	×	1.79	–0.88	0.90	DFPT incomplete		
$La_{10}Se_{14}O$	$I4_1/acd$	8.3 (O-2p)	1.59	–0.63	0.96	1.60	–0.64	0.96
$La_4Mo_2O_{11}$	$P4_2/n$	×	DFT incomplete			×	×	×
$La_4Se_3O_4$	$Amm2$	6.3 (O-2p)	2.01	–0.34	1.67	2.04	–0.36	1.68
$La_6BN_3O_6$	$Cmcm$	6.5 (N-2p), 8.4 (O-2p)	1.10	0.20	1.29	1.81	–0.16	1.65
$LaCuS_2$	$P2_1/c$	14.7 (Cu-3d)	1.20	–0.23	0.97	1.75	–0.50	1.25
LaCuSeO	$P4/nmm$	15.6 (Cu-3d), 8.3 (O-2p)	1.48	–0.20	1.29	2.44	–0.68	1.76
LaCuSO	$P4/nmm$	15.5 (Cu-3d), 8.3 (O-2p)	1.70	–0.24	1.46	2.65	–0.71	1.94
LaSO	$Cmce$	8.3 (O-2p)	1.56	0.04	1.60	1.57	0.03	1.61
$LaTiNO_2$	$I2_12_12_1$	5.9 (Ti-3d), 6.4 (N-2p), 8.4 (O-2p)	1.36	0.24	1.60	2.42	–0.28	2.13
Li_2MnBr_4	$Cmmm$	×	1.86	–0.11	1.75	DFT incomplete		
$Li_3V_2P_3O_{12}$	$P2_1/c$	×	0.03	1.38	1.42	DFT incomplete		
$LiCoO_2$	$R\bar{3}m$	6.1 (Co-3d), 8.4 (O-2p)	1.11	0.21	1.32	0.01	0.76	0.77
LiCuO	$I4/mmm$	12.4 (Cu-3d), 9.0 (O-2p)	1.49	–0.52	0.97	2.42	–0.98	1.44
$LiVO_2$	$R\bar{3}m$	3.8 (V-3d), 8.7 (O-2p)	0.01	0.54	0.54	2.26	–0.59	1.67
MgB_9N	$R\bar{3}m$	6.2 (N-2p)	1.68	–0.83	0.85	1.96	–0.97	0.99
$MgFe_2O_4$	$Fd\bar{3}m$	×	0.01	1.27	1.28	DFT incomplete		
$MgMoN_2$	$P6_3/mmc$	6.8 (N-2p), 3.4 (Mo-4d)	0.90	0.39	1.29	0.71	0.49	1.20
$MgTe_2$	$Pa\bar{3}$	None	1.08	–0.15	0.94	—	—	—
$Mn_3V_2O_8$	$I\bar{4}$	8.2 (Mn-3d), 5.9 (V-3d), 8.2 (O-2p)	0.65	0.95	1.6	0.71	0.92	1.63
$MnGa_2S_4$	$I\bar{4}$	6.6 (Mn-3d)	1.25	–0.28	0.96	2.28	–0.8	1.48
MnO	$R\bar{3}m$	7.0 (Mn-3d), 8.0 (O-2p)	0.01	0.85	0.86	2.30	–0.29	2.00
Mo_6PbI_{14}	$Pn\bar{3}$	×	1.84	0.27	2.11	DFT incomplete		
MoS_2	$R3m$	3.7 (Mo-4d)	1.51	0.13	1.64	1.46	0.15	1.62
$MoSe_2$	$P\bar{3}m1$	3.8 (Mo-4d)	1.44	–0.02	1.41	1.24	0.07	1.32
$Na_2Sn_2Se_5$	$Pbca$	None	1.03	–0.28	0.75	—	—	—
Na_2TeO_4	$P2_1/c$	8.7 (O-2p)	1.39	0.32	1.71	3.30	–0.63	2.67
Na_3BiO_4	$P2/c$	9.6 (O-2p)	1.04	0.35	1.39	2.21	–0.24	1.98
$Na_3Fe_5O_9$	$C2/c$	6.3 (Fe-3d), 8.7 (O-2p)	0.00	0.85	0.86	3.57	–0.93	2.64
$Na_3Mn_4Te_2O_{12}$	$Pnma$	8.3 (Mn-3d), 8.6 (O-2p)	0.05	1.10	1.15	DFT+U incomplete		

	Space group	U parameters (eV)	DFT			DFT+U		
			ε_g (eV)	eE_{CB} (eV)	eE_{VB} (eV)	ε_g (eV)	eE_{CB} (eV)	eE_{VB} (eV)
Na_3WN_3	*Cc*	3.3 (W-5*d*), 6.3 (N-2*p*)	1.80	–0.80	1.00	2.37	–1.09	1.29
$Na_4Fe_2O_5$	$P2_1/c$	6.5 (Fe-3*d*), 8.6 (O-2*p*)	0.03	0.27	0.31	3.80	–1.61	2.19
$Na_4VP_2O_9$	*Pbca*	×	DFT incomplete			×	×	×
Na_5CoHO_4	*Pnma*	×	DFT incomplete			×	×	×
$Na_5CuH_2O_4$	*Pnma*	13.0 (Cu-3*d*), 10.0 (O-2*p*)	1.49	–0.41	1.08	3.64	–1.48	2.16
Na_5NiO_4	*Pbca*	×	0.53	–0.31	0.22	DFT incomplete		
$NaInO_2$	$R\bar{3}m$	8.5 (Mo-4*d*)	1.92	–0.67	1.26	4.22	–1.81	2.4
$NaMnO_2$	$C2/m$	4.9 (Mn-3*d*), 8.3 (O-2*p*)	1.16	–0.07	1.10	2.60	–0.78	1.81
$NaMo_6Br_{13}$	$P\bar{1}$	3.7 (Mo-4*d*)	2.19	0.39	2.57	2.54	0.21	2.75
$NaNbO_2$	$P6_3/mmc$	1.9 (Nb-4*d*), 9.1 (O-2*p*)	1.43	–0.11	1.32	2.07	–0.43	1.64
$Nb_3Sb_2Te_5$	$I\bar{4}3m$	2.9 (Nb-4*d*)	0.81	0.02	0.84	0.72	0.07	0.79
$NbCu_3S_4$	$P\bar{4}3m$	2.9 (Nb-4*d*), 13.9 (Cu-3*d*)	1.81	–0.14	1.67	1.97	–0.22	1.75
$Pb_5S_2I_6$	$C2/m$	None	1.89	0.02	1.91	1.89	0.02	1.91
PbO	*Pbcm*	8.1 (O-2*p*)	1.81	0.08	1.89	2.83	–0.43	2.40
Rb_2MnCl_4	$C2/m$	6.7 (Mn-3*d*)	1.34	0.04	1.39	3.70	–1.14	2.56
Rb_2NaMnO_4	$P2_1/m$	8.2 (Mn-3*d*), 8.9 (O-2*p*)	1.23	–0.49	0.74	1.08	–0.42	0.66
$Rb_4Cu_5Cl_9$	*Pc*	×	DFT incomplete			×	×	×
$Rb_4P_{21}I$	*Cmcm*	None	1.39	–0.19	1.20	—	—	—
$Rb_4Ta_2S_{11}$	$Pca2_1$	2.7 (Ta-5*d*)	1.75	–0.61	1.14	DFT+U incomplete		
$Rb_4Ti_3S_{14}$	$C2/c$	5.4 (Ti-3*d*)	1.27	–0.33	0.94	2.11	–0.75	1.36
$Rb_4Zr_3Se_{14}$	$C2/c$	2.6 (Zr-4*d*)	1.50	–0.58	0.92	1.67	–0.66	1.01
$Rb_6Ta_4S_{25}$	*P*1	2.7 (Ta-5*d*)	1.47	–0.16	1.31	1.47	–0.16	1.31
$RbCuO_2$	*Cmcm*	11.2 (Cu-3*d*), 8.1 (O-2*p*)	1.03	–0.01	1.01	2.23	–0.61	1.62
Sb_2S_3	*Pnma*	None	1.31	0.54	1.85	—	—	—
$SbPb_2S_2I_3$	$P2_1/c$	None	1.81	0.19	2.00	—	—	—
SiP	$Cmc2_1$	None	1.75	–0.14	1.62	—	—	—
SiP_2	*Pbam*	None	1.42	0.17	1.59	—	—	—
SnS	*Pnma*	None	1.14	0.16	1.30	—	—	—
SnS_2	$P\bar{3}m1$	None	1.53	0.30	1.83	—	—	—
$Sr_{17}Ta_{10}S_{42}$	*P*1	×	DFT incomplete			×	×	×

	Space group	U parameters (eV)	DFT			DFT+U		
			ε_g (eV)	eE_{CB} (eV)	eE_{VB} (eV)	ε_g (eV)	eE_{CB} (eV)	eE_{VB} (eV)
$Sr_2Fe_2S_2OF_2$	*I*4/*mmm*	6.9 (Fe-3*d*), 8.9 (O-2*p*)	0.07	0.56	0.63	0.19	0.50	0.69
Sr_2FeBrO_3	*P*4/*nmm*	7.4 (Fe-3*d*), 8.9 (O-2*p*)	0.04	0.27	0.31	3.17	–1.30	1.87
Sr_2FeClO_3	*P*4/*nmm*	7.2 (Fe-3*d*), 8.9 (O-2*p*)	0.05	0.32	0.37	3.18	–1.24	1.94
Sr_2FeO_3F	*P*4/*nmm*	7.6 (Fe-3*d*), 9.0 (O-2*p*)	0.04	0.49	0.53	3.07	–1.03	2.04
Sr_2PbO_4	*Pbam*	9.0 (O-2*p*)	1.43	–0.46	0.97	2.31	–0.90	1.41
$Sr_2SnSe_3F_2$	*Pnma*	None	1.45	–0.18	1.27	—	—	—
$Sr_4Mn_3O_{10}$	*P*222$_1$	7.2 (Mn-3*d*), 9.0 (O-2*p*)	0.91	–0.02	0.89	0.69	0.08	0.78
$Sr_6Sb_6S_{17}$	*P*2$_1$2$_1$2$_1$	×	DFT incomplete			×	×	×
$SrCu_2O_2$	*I*4$_1$/*amd*	12.8 (Cu-3*d*), 8.3 (O-2*p*)	1.81	–0.65	1.16	3.11	–1.30	1.81
SrCuSeF	*P*4/*nmm*	16.2 (Cu-3*d*)	1.15	–0.17	0.98	2.26	–0.73	1.53
SrCuSF	*P*4/*nmm*	16.1 (Cu-3*d*)	1.45	–0.26	1.20	2.73	–0.89	1.83
$SrIn_2O_4$	*Pnma*	8.8 (O-2*p*)	1.83	–0.52	1.31	3.93	–1.56	2.36
Te_2Mo	*P*6$_3$/*mmc*	3.6 (Mo-4*d*)	1.01	–0.05	0.96	0.93	0.00	0.92
$TiPbO_3$	*P*4*mm*	6.3 (Ti-3*d*), 8.1 (O-2*p*)	2.08	0.17	2.25	3.45	–0.51	2.94
$V_5Pb_2O_{12}$	*P*2/*c*	5.7 (V-3*d*), 7.8 (O-2*p*)	0.49	1.11	1.60	2.75	–0.02	2.72
VCu_3Se_4	*P*$\bar{4}$3*m*	5.1 (V-3*d*), 13.2 (Cu-3*d*)	0.99	0.06	1.05	1.40	–0.14	1.26
VO	*Fm*$\bar{3}$*m*	×	DFT incomplete			×	×	×
WS_2	*P*6$_3$/*mmc*	3.2 (W-5*d*)	1.66	0.27	1.93	1.71	0.25	1.96
WSe_2	*P*6$_3$/*mmc*	3.2 (W-5*d*)	1.52	0.14	1.67	1.36	0.23	1.59
$YCuS_2$	*Pnma*	15.1 (Cu-3*d*)	1.63	–0.41	1.23	2.18	–0.68	1.50
$ZnCo_2O_4$	*F*d$\bar{3}$*m*	×	DFT incomplete			×	×	×
$ZnFe_2O_4$	*Fd*$\bar{3}$*m*	15.3 (Zn-3*d*), 6.2 (Fe-3*d*), 8.6 (O-2*p*)	0.01	1.41	1.43	3.60	–0.38	3.22
$ZnGeP_2$	*I*$\bar{4}$2*d*	None	1.27	–0.03	1.24	—	—	—
ZnP_2	*P*4$_3$2$_1$2	None	1.50	0.01	1.51	—	—	—
ZnSe	*F*$\bar{4}$3*m*	None	1.47	–0.05	1.42	—	—	—
ZnTe	*F*$\bar{4}$3*m*	None	1.32	–0.16	1.16	—	—	—

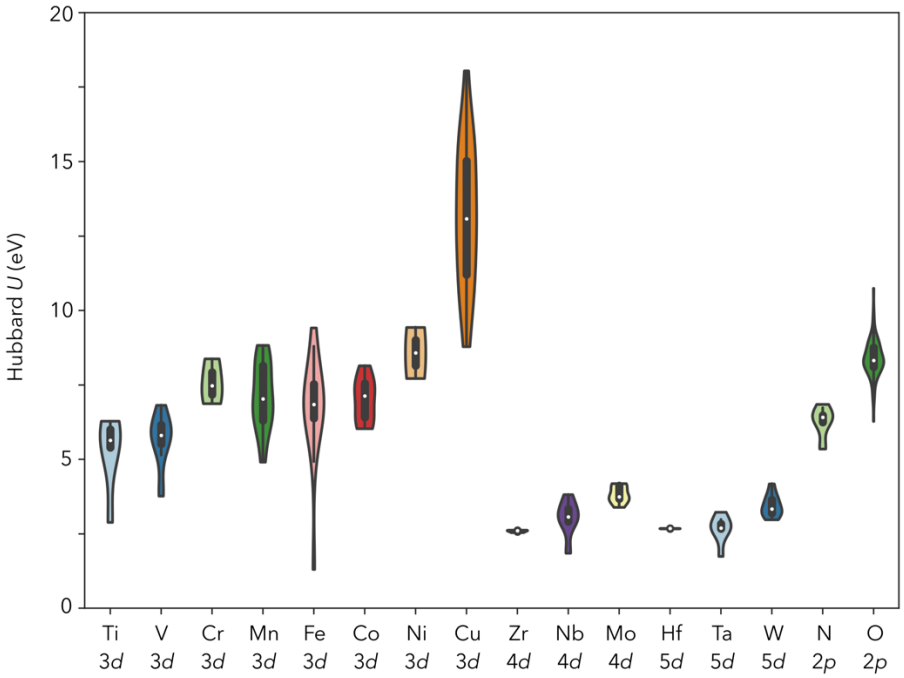


Figure S3 Distributions of the Hubbard *U* parameters for the transition-metal, carbon, nitrogen and oxygen elements. The *U* parameters are computed from first principles using DFPT,[1] with orthogonalized atomic orbitals as projectors on the Hubbard manifold. The distributions illustrate the gradual increase in the *U* parameters across the transition-metal series, following electronegativity trends. It is noted that the *U* parameters of Cu present higher values compared to other elements. This observation is due to the fact that the Cu-3*d* electronic shell is closed.[4] The variance of the *U* parameters is the largest for iron and copper cations. In contrast, the distribution of *U* parameters of the oxygen anion is narrow. In light of this statistical results, we performed a sensitivity analysis of the computed band gap ε_g as a function of the *U* parameter for the cuprous compounds (listed in Table 2 of the main text), finding an average decrease in ε_g of 0.09 eV when reducing *U*(Cu-3*d*) by 1 eV. Cu_2WS_4 and $Na_5CuH_2O_4$ exhibited the lowest sensitivity (0.03 eV per 1 eV) and highest sensitivity (0.16 eV per 1 eV) to the *U*(Cu-3*d*) parameter, respectively. This assessment suggests that although the *U*(Cu-3*d*) parameters are quite large and widely distributed, they do not translate into unexpectedly strong or unreasonably sensitive Hubbard *U* corrections to the original (DFT) band gaps.

[4] Yu, Carter, *The Journal of Chemical Physics* **140**, 121105 (2014).

Table S2 Identification number, formation energies, and band gaps from the Materials Project (MP) for the 162 candidate photocatalysts. The formation energies and band gaps are evaluated at the DFT/DFT+U level with fixed U parameters (DFT+U_{MP}) using the VASP (Vienna Ab initio Simulation Package) code.[5,6] The U_{MP} parameters are optimally tuned to reproduce experimental formation enthalpies: 3.3 (V-3*d*), 3.7 (Cr-3*d*), 3.9 (Mn-3*d*), 5.3 (Fe-3*d*), 3.3 (Co-3*d*), 6.2 eV (Ni-3*d*).[7,8] It is important to note that some of the U_{MP} parameters are far from those computed in this work from first principles. This is because U depends on numerical and physical parameters, such as the pseudopotentials [GBRV ultrasoft pseudopotentials[9] are used in this work, while projected augmented-wave (PAW) pseudopotentials[10] are used in the Materials Project], the localized functions of the Hubbard projectors (orthogonalized atomic orbitals are used in this work while PAW projector functions are used in VASP), and the chemical environments of the elements. Hence, U is in general not transferable. The elements in the chemical formula are ordered by increasing electronegativity, following the naming convention of the Materials Project.

	Space group	MP identity number	Formation energy (eV/atom)	DFT+U_{MP} ε_g (eV)
$AlCuO_2$	$R\bar{3}m$	3748	–2.42	1.82
$Ba_2Fe_2O_5$	$P2_1/c$	1196071	–2.41	1.42
$Ba_2In_2S_5$	$Pbca$	22841	–1.67	1.99
Ba_2PbO_4	$I4/mmm$	20098	–2.38	1.22
$Ba_2SnSe_3F_2$	$Pnma$	17805	–2.26	1.72
$Ba_3MnNb_2O_9$	$P\bar{3}m1$	20921	–3.14	1.77
$Ba_3Zn_5In_2O_{11}$	$F\bar{4}3m$	560544	–2.19	1.62
$Ba_6Mn_5O_{16}$	$Cmce$	30895	–2.42	1.30
$Ba_6V_4S_{11}O_5$	$Pnma$	556461	–2.09	1.91
$Ba_8Sb_6S_{17}$	$P2/c$	561455	–1.62	1.39
$BaAlSi_5N_7O_2$	$P1$	1227994	–1.82	1.51
$BaCaFe_4O_8$	$P\bar{3}1m$	18950	–1.43	1.78
$BaCu_2O_2$	$I4_1/amd$	7374	–1.62	1.38
$BaHfN_2$	$P4/nmm$	10322	–1.53	1.25
$BaIn_2O_4$	$P2_1/c$	578629	–2.27	1.67
BaS_2	$C2/c$	684	–1.86	1.58
$BaSbSe_2F$	$P\bar{1}$	558946	–1.81	1.33
$BaSnS_2$	$P2_1/c$	12181	–1.63	1.64
$Ca_{12}Al_{14}O_{33}$	$C2$	530149	–3.45	1.97
Ca_2CoO_3	Cm	1182074	–2.45	1.75

[5] Kresse, Furthmüller, *Computational Materials Science* **6**, 15-50 (1996).
[6] Kresse, Furthmüller, *Physical Review B* **54**, 11169 (1996).
[7] Jain *et al.*, *Physical Review B* **84**, 045115 (2011).
[8] Wang, Maxisch, Ceder, *Physical Review B* **73**, 195107 (2006).
[9] Garrity, Bennett, Rabe, Vanderbilt, *Computational Materials Science* **81**, 446-452 (2014).
[10] Kresse, Joubert *Physical Review B* **59**, 1758 (1999).

	Space group	MP identity number	Formation energy (eV/atom)	DFT+U_{MP} ε_g (eV)
Ca_2FeClO_3	$P4/nmm$	630511	–2.41	0.99
Ca_2PbO_4	$Pbam$	21137	–2.56	1.48
Ca_3PCl_3	$Pm\bar{3}m$	29342	–2.27	1.84
$CaFeClO_2$	$C2/m$	549711	–2.00	2.00
$CaIn_2O_4$	$Fd\bar{3}m$	22766	–2.40	1.92
$CaSb_{10}S_6O_{10}$	$C2/c$	504882	–1.49	1.75
$CaTaNO_2$	$Pmc2_1$	556340	–2.76	1.61
$CoPb_2WO_6$	$C2/m$	20069	–1.78	1.78
Cr_3BO_6	$Pnma$	18551	–2.32	1.60
$CrPb_5O_8$	$P2_1/c$	705034	–1.61	1.88
$Cs_4Ta_2S_{11}$	$Pca2_1$	14578	–1.39	1.81
$Cs_4Ti_3S_{14}$	$C2/c$	542011	–1.46	1.29
$Cs_4Zr_3Se_{14}$	$C2/c$	768674	–1.05	1.51
$CsCuO_2$	$Cmcm$	553310	–1.36	0.94
$CsGeI_3$	$R3m$	28377	–0.83	1.59
$CsLaNb_2O_7$	$P4/mmm$	553248	–3.21	1.44
$CsMnBr_3$	$P6_3/mmc$	23048	–0.82	1.29
$CsMnI_3$	$P6_3/mmc$	540609	–0.47	1.02
$CsSbS_2$	$P2_1/c$	561639	–1.05	1.84
Cu_2WS_4	$P\bar{4}2m$	8976	–0.84	1.45
Cu_3SbS_3	$P2_12_12_1$	17691	–0.48	1.00
CuI	$P3m1$	570136	–0.15	1.63
CuP_2	$P2_1/c$	927	–0.11	0.86
Fe_3BO_6	$Pnma$	22774	–1.61	1.79
$FeNi_2BO_5$	$Pbam$	21522	–1.76	1.85
Ga_2TeSe_2	$I4_1md$	28423	–0.51	1.61
$GaCuI_4$	$I\bar{4}$	29403	–0.41	1.70
$GaCuO_2$	$R\bar{3}m$	4280	–1.68	0.98
GaN	$P6_3mc$	804	–0.67	1.74
GaS	$P6_3/mmc$	2507	–0.98	1.88

	Space group	MP identity number	Formation energy (eV/atom)	DFT+U_{MP} ε_g (eV)
Ge_4Se_9	$Pca2_1$	680333	–0.21	1.22
GeI_4	$Pa\bar{3}$	23266	–0.27	2.00
GeS	$Pnma$	2242	–0.58	1.24
GeSe	$Pnma$	700	–0.17	0.90
$GeSe_2$	$P2_1/c$	540625	–0.23	1.44
GeTe	$R3m$	938	–0.09	0.75
In_2O_3	$I2_13$	22598	–2.01	0.93
$In_4Bi_2S_9$	$P2_1/m$	27195	–0.87	1.63
InBr	$Cmcm$	22870	–0.67	1.26
InI	$Cmcm$	23202	–0.47	1.34
$InSb_2S_4Br$	$C2/m$	559864	–0.75	1.52
$InSb_2S_4Cl$	$C2/m$	556541	–0.87	1.51
$InSb_2Se_4Br$	$P\bar{1}$	570321	–0.41	1.13
K_2CoCl_4	$Pna2_1$	23515	–1.74	0.89
K_2NbCuS_4	$Fddd$	9763	–1.38	1.96
$K_2TaCuSe_4$	$Fddd$	8972	–0.95	1.98
$K_3LaP_2Se_8$	P_1/c	542079	–0.93	1.46
K_3P_{11}	$Pbcn$	1568	–0.32	1.93
K_3PSe_{16}	Fd–3	29947	–0.34	1.09
K_3PSe_4	$Pnma$	31313	–0.87	1.83
$K_3VP_2O_8$	$P2_1$/c	557046	–2.54	1.98
$K_4P_{21}I$	$Cmcm$	31280	–0.30	1.34
$KBiP_2Se_6$	$P2_1/c$	569435	–0.40	1.61
$KCoO_2$	$I\bar{4}$	1180771	–1.58	0.99
$KCuO_2$	$Cmcm$	3982	–1.39	0.86
$KLa_5C_2Cl_{10}$	$P2_1/c$	571240	–2.32	1.94
$KNaZnO_2$	$C2/c$	557183	–1.64	1.78
$KV_3P_4O_{17}$	$P2_12_12_1$	14929	–2.61	1.16
$La_{10}Se_{14}O$	$I4_1/acd$	558535	–2.18	1.55
$La_4Mo_2O_{11}$	$P4_2/n$	14748	–3.18	1.82

	Space group	MP identity number	Formation energy (eV/atom)	DFT+U_{MP} ε_g (eV)
$La_4Se_3O_4$	*Amm*2	4412	–3.13	1.33
$La_6BN_3O_6$	*Cmcm*	560824	–3.02	1.10
$LaCuS_2$	$P2_1/c$	4841	–1.80	1.23
LaCuSeO	*P*4/*nmm*	552488	–2.20	1.55
LaCuSO	*P*4/*nmm*	6088	–2.40	1.67
LaSO	*Cmce*	28626	–3.11	1.52
$LaTiNO_2$	$I2_12_12_1$	1222738	–3.06	1.21
Li_2MnBr_4	*Cmmm*	28250	–1.23	1.78
$Li_3V_2P_3O_{12}$	$P2_1/c$	757321	–2.71	1.92
$LiCoO_2$	$R\bar{3}m$	22526	–1.59	0.66
LiCuO	*I*4/*mmm*	5127	–1.44	1.44
$LiVO_2$	$R\bar{3}m$	19340	–2.50	1.79
MgB_9N	$R\bar{3}m$	30091	–0.43	1.68
$MgFe_2O_4$	$Fd\bar{3}m$	608016	–2.25	1.80
$MgMoN_2$	$P6_3/mmc$	864954	–1.06	0.74
$MgTe_2$	$Pa\bar{3}$	2604	–0.58	1.12
$Mn_3V_2O_8$	$I\bar{4}$	1221916	–2.28	1.92
$MnGa_2S_4$	$I\bar{4}$	20025	–1.04	1.18
$MnNi_6O_8$	$Fm\bar{3}m$	19442	–1.22	1.31
MnO	$R\bar{3}m$	19006	–1.99	1.68
Mo_6PbI_{14}	$Pn\bar{3}$	569225	–0.44	1.84
MoS_2	*R*3*m*	1434	–1.31	1.20
$MoSe_2$	$P\bar{3}m1$	1027692	–0.67	1.14
$Na_2Sn_2Se_5$	*Pbca*	16167	–0.63	1.02
Na_2TeO_4	$P2_1/c$	560613	–1.83	1.81
Na_3BiO_4	*P*2/*c*	27345	–1.74	0.96
$Na_3Fe_5O_9$	*C*2/*c*	540658	–1.34	1.72
$Na_3Mn_4Te_2O_{12}$	*Pnma*	561325	–1.93	1.45
Na_3WN_3	*Cc*	16839	–0.63	1.77
$Na_4Fe_2O_5$	$P2_1/c$	19396	–1.34	1.92

	Space group	MP identity number	Formation energy (eV/atom)	DFT+U_{MP} ε_g (eV)
$Na_4VP_2O_9$	*Pbca*	705037	–2.61	1.76
Na_5CoHO_4	*Pnma*	774341	–1.49	1.68
$Na_5CuH_2O_4$	*Pnma*	757878	–1.49	1.49
Na_5NiO_4	*Pbca*	21996	–1.39	1.91
$NaInO_2$	$R\bar{3}m$	5175	–2.00	1.91
$NaMnO_2$	*C*2/*m*	18957	–2.04	1.26
$NaMo_6Br_{13}$	$P\bar{1}$	680472	–0.77	2.00
$NaNbO_2$	$P6_3/mmc$	3744	–2.54	1.38
$Nb_3Sb_2Te_5$	$I\bar{4}3m$	569571	–0.40	0.84
$NbCu_3S_4$	$P\bar{4}3m$	5621	–0.93	1.66
$Pb_5S_2I_6$	*C*2/*m*	23066	–0.70	1.81
PbO	*Pbcm*	672237	–1.48	1.47
Rb_2MnCl_4	*C*2/*m*	22978	–1.94	1.29
Rb_2NaMnO_4	$P2_1/m$	18873	–1.83	1.81
$Rb_4Cu_5Cl_9$	*Pc*	29449	–1.41	1.79
$Rb_4P_{21}I$	*Cmcm*	31279	–0.31	1.43
$Rb_4Ti_3S_{14}$	*C*2/*c*	542067	–1.45	1.22
$Rb_4Zr_3Se_{14}$	*C*2/*c*	542013	–1.03	1.46
$Rb_6Ta_4S_{25}$	*P*1	680284	–1.26	1.48
$RbCuO_2$	*Cmcm*	7467	–1.37	0.91
Sb_2S_3	*Pnma*	2809	–0.65	1.28
$SbPb_2S_2I_3$	$P2_1/c$	578882	–0.66	1.72
SiP	$Cmc2_1$	2798	–0.14	1.74
SiP_2	*Pbam*	9996	–0.13	1.42
SnS	*Pnma*	2231	–0.78	0.91
SnS_2	$P\bar{3}m1$	1170	–0.82	1.56
$Sr_{17}Ta_{10}S_{42}$	*P*1	532315	–1.96	1.79
$Sr_2Fe_2S_2OF_2$	*I*4/*mmm*	549237	–2.55	1.90
Sr_2FeBrO_3	*P*4/*nmm*	556507	–2.56	1.35
Sr_2FeClO_3	*P*4/*nmm*	630641	–2.72	1.12

	Space group	MP identity number	Formation energy (eV/atom)	DFT+U_{MP} ε_g (eV)
Sr_2FeO_3F	*P*4/*nmm*	19293	–2.96	1.20
Sr_2PbO_4	*Pbam*	20944	–2.48	1.40
$Sr_2SnSe_3F_2$	*Pnma*	17057	–2.23	1.45
$Sr_4Mn_3O_{10}$	$P222_1$	18998	–2.60	1.30
$Sr_6Sb_6S_{17}$	$P2_12_12_1$	16061	–1.43	1.74
$SrCu_2O_2$	$I4_1/amd$	13900	–1.67	1.81
SrCuSeF	*P*4/*nmm*	21228	–2.15	1.20
SrCuSF	*P*4/*nmm*	12444	–2.35	1.51
$SrIn_2O_4$	*Pnma*	540688	–2.37	1.81
Te_2Mo	$P6_3/mmc$	602	–0.27	0.97
$TiPbO_3$	*P*4*mm*	20459	–2.74	1.82
$V_5Pb_2O_{12}$	*P*2/*c*	22296	–2.29	1.82
VCu_3Se_4	$P\bar{4}3m$	21855	–0.49	0.82
VO	$Fm\bar{3}m$	19184	–2.09	0.78
WS_2	$P6_3/mmc$	224	–1.26	1.56
WSe_2	$P6_3/mmc$	1821	–0.56	1.45
$YCuS_2$	*Pnma*	10533	–1.70	1.60
$ZnCo_2O_4$	$Fd\bar{3}m$	753489	–1.49	1.94
$ZnFe_2O_4$	$Fd\bar{3}m$	19313	–1.89	1.67
$ZnGeP_2$	$I\bar{4}2d$	4524	–0.21	1.17
ZnP_2	$P4_32_12$	11025	–0.25	1.46
ZnSe	$F\bar{4}3m$	1190	–0.72	1.17
ZnTe	$F\bar{4}3m$	2176	–0.47	1.08

S4. Tauc measurements of band gaps

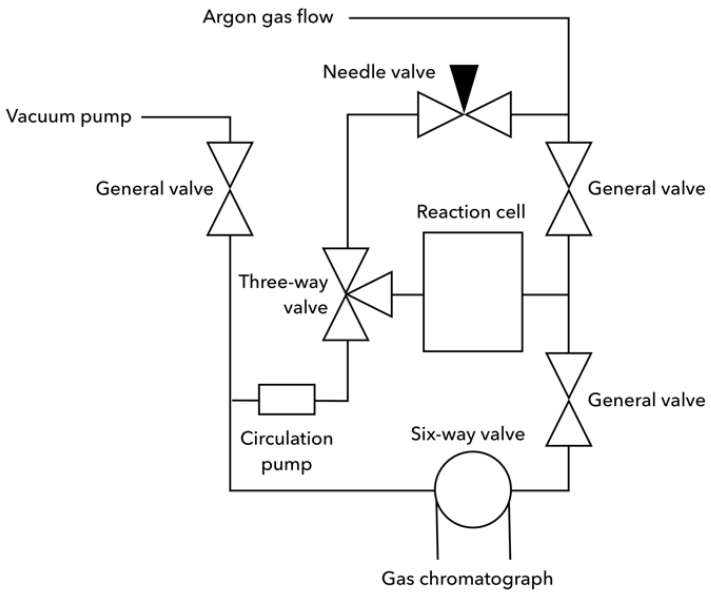
The band gaps of the synthesized compounds were determined using diffuse reflectance with a UV-visible spectrophotometer, as described in the Materials Characterization section in the main text. The results of the Tauc measurements are summarized in Fig. S2. Most of the samples showed a clear transition in the Tauc plot; however, multiple transitions were found for some of the compounds, most notably for $BaCaFe_4O_6$, which indicates the presence of mid-gap states, potentially due to defects.

S5. Mott–Schottky measurements of band edges

To determine the band edges of the synthesized materials, Mott–Schottky measurements were performed in an aqueous solution with a sodium phosphate buffer electrolyte at pH 8, and with the room's lights turned off. The measurements were performed for different frequencies over a range of potentials at constant frequency. The flatband potentials were averaged across these different frequencies to obtain the values reported in Table 1 of the main text. The Mott–Schottky plots of the compounds are shown in Fig. S3.

S6. Gas chromatography measurements

Hydrogen evolution tests were carried out using a gas chromatography setup depicted below:



Measurements were performed using a HP 5890 Series II gas chromatograph with a thermal conductivity detector under argon carrier gas. The setup can operate in continuous-flow and accumulation-flow modes. Under continuous flow, the argon supply was controlled by a needle valve and the generated gas was tested continuously by the gas chromatograph. In accumulation mode, the produced gas was stored for a period of time before being transferred to the gas chromatograph by the circulation pump. In this work, hydrogen evolution data were collected in the accumulation mode. The results of the gas chromatography are plotted in Fig. S5. The gas chromatograph was calibrated *via* needle injection of a known volume of gas.

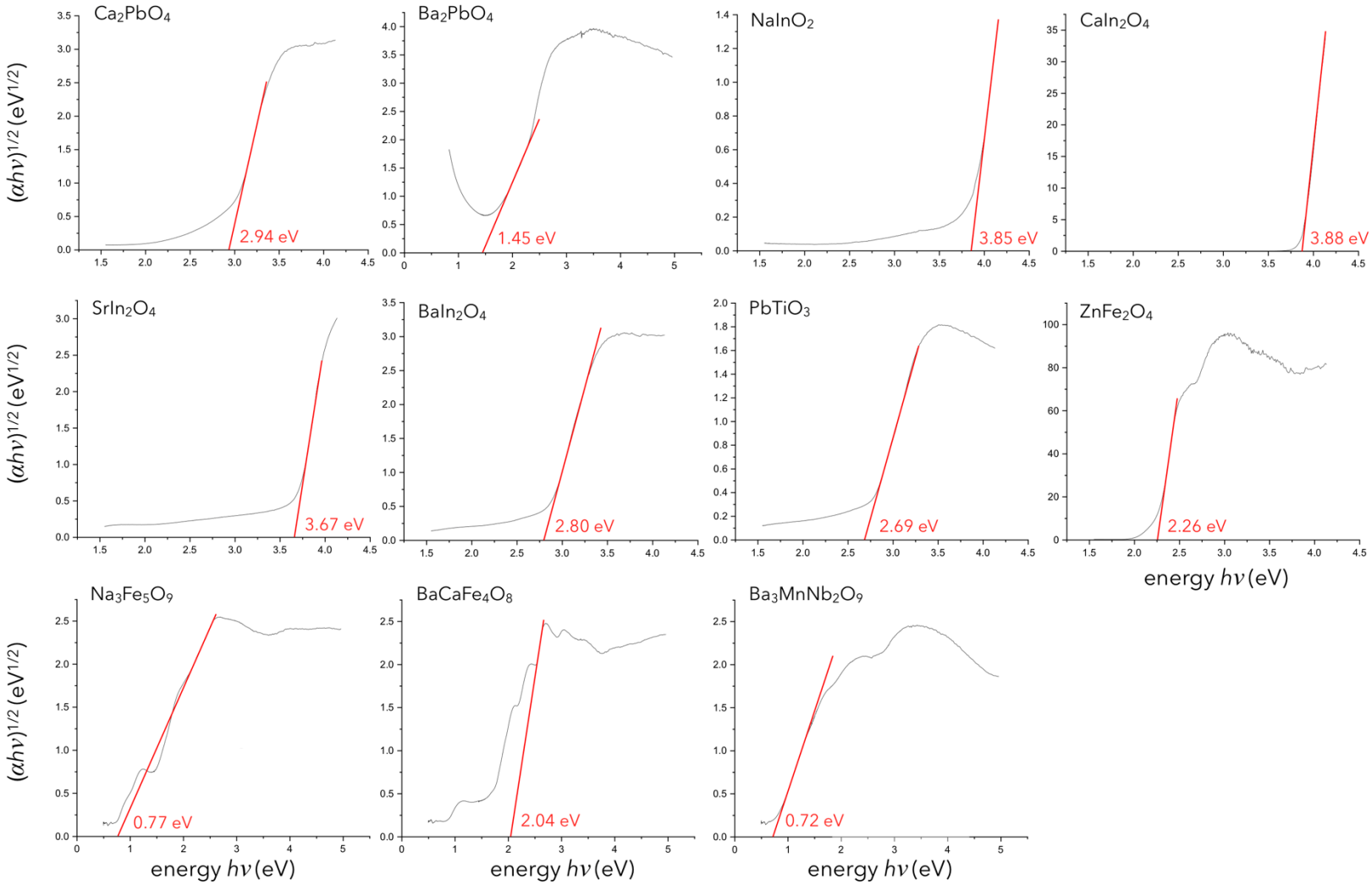


Figure S4 Tauc plots of the synthesized compounds. The band gaps of the materials were determined by linear extrapolation of the Tauc signal. The light absorption coefficient and energy of the incident photon are denoted as α and $h\nu$, respectively.

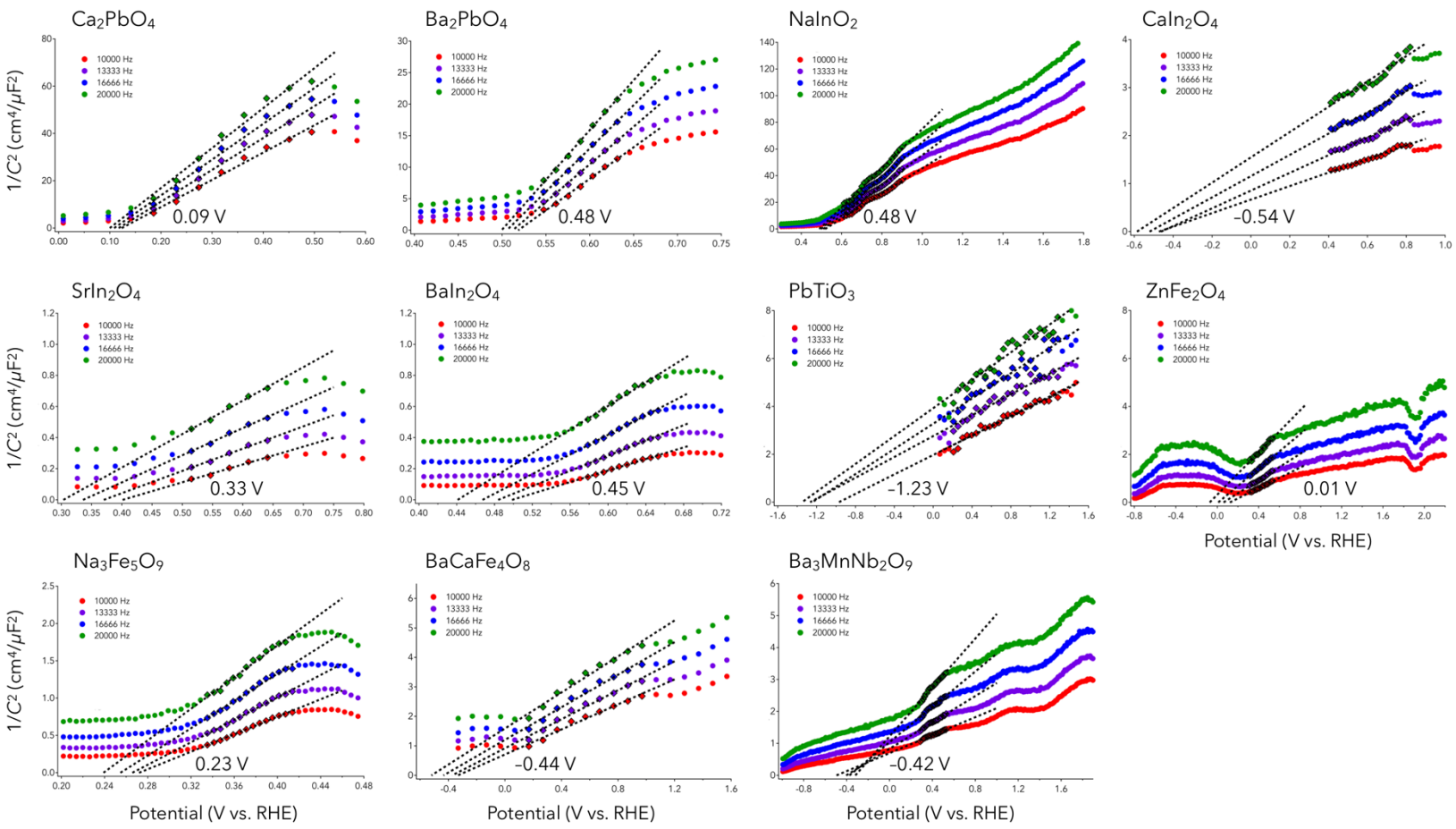


Figure S5 Mott–Schottky analysis of the synthesized compounds. The measurements were performed in an aqueous sodium phosphate buffer solution at pH 8, and under dark conditions. Following the Mott–Schottky equation, the flatband potentials E_{FB} were determined as $E_0 - k_B T/e = E_0 - 0.025$ V where E_0 denotes the intercept of the linearly extrapolated inverse squared capacitance with the horizontal axis, averaged over frequencies.

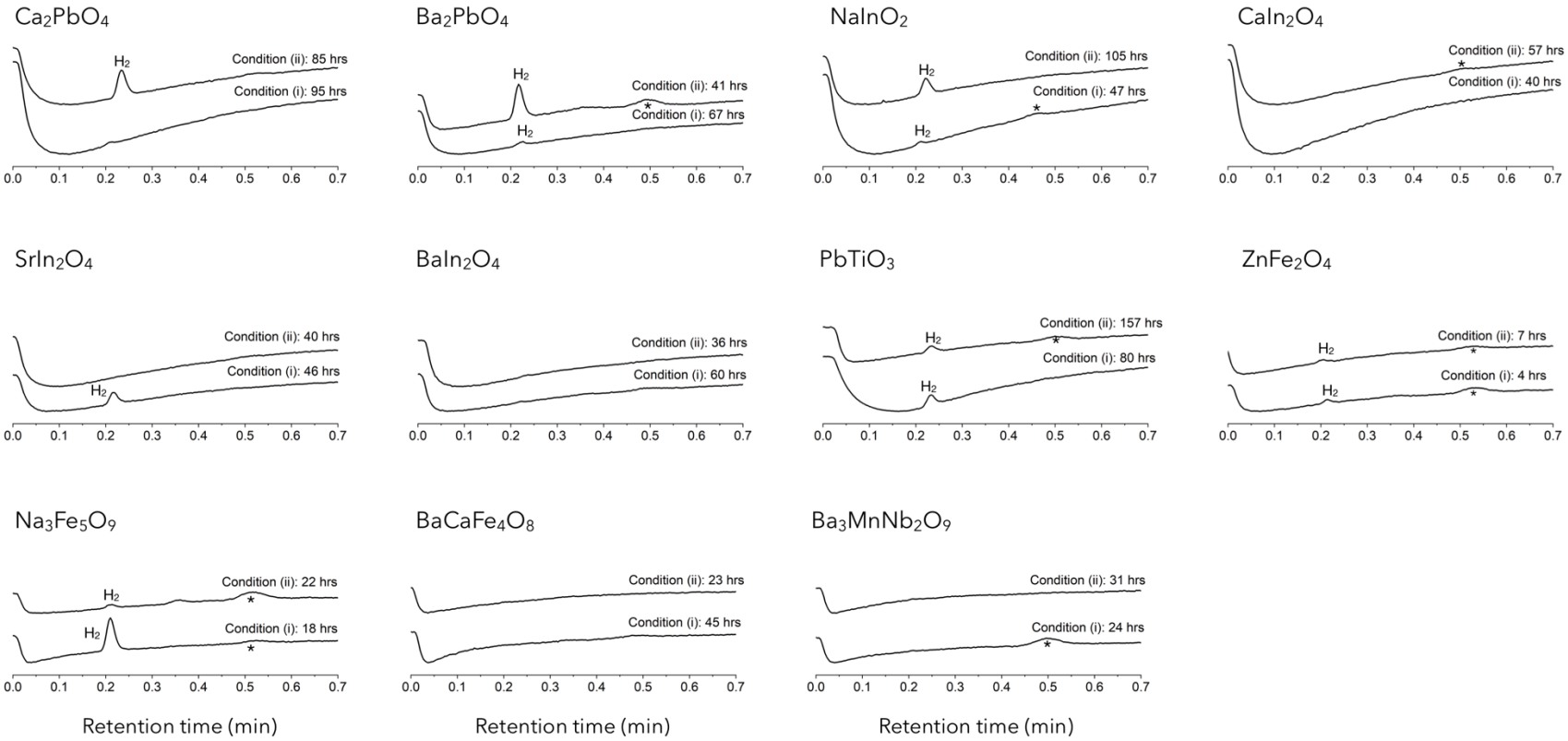
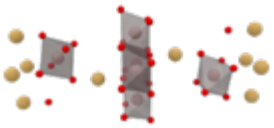
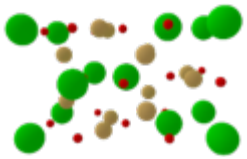
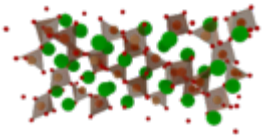
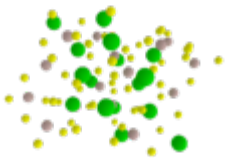
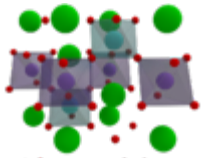
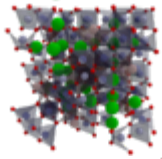
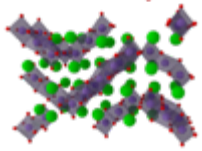
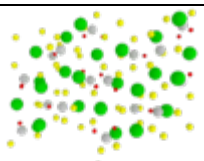
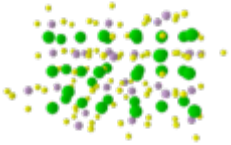
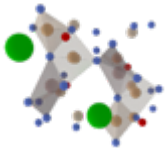
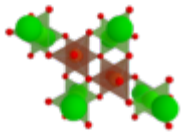
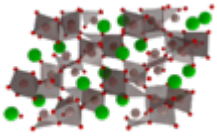
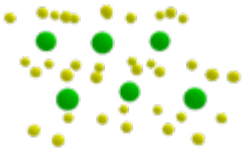
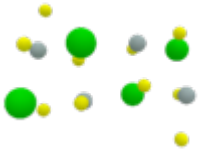
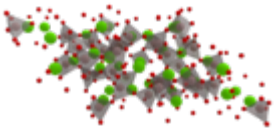


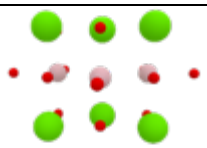
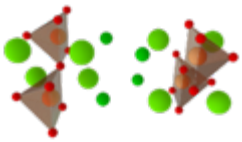
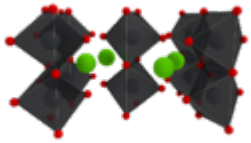
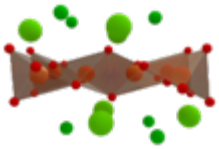
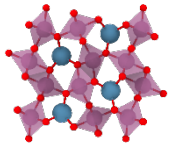
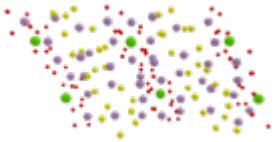
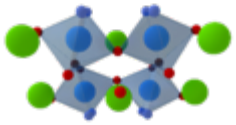
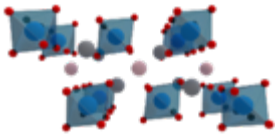
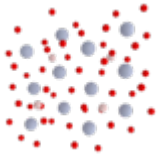
Figure S6 Gas chromatography measurements of the synthesized compounds for water-splitting applications. Measurements were performed under condition (*i*) with 0.1 M oxalic acid solution and under condition (*ii*) with a volume fraction of 15% of methanol in water, as described in the main text. The retention times are given in fraction of a minute (0.1 minute means 6 seconds). The moderate drifts in the hydrogen baseline are due to slight fluctuations in the pressure of argon in the instrument. The asterisks (*) indicate nitrogen that possibly originates from traces of air remaining in the chamber but was not found to affect hydrogen detection.

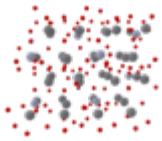
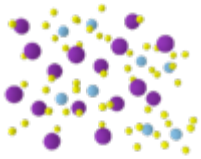
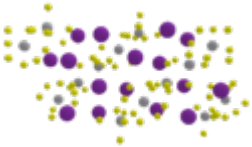
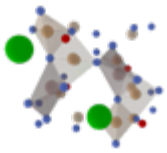
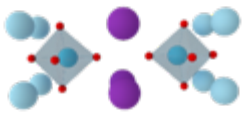
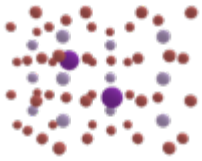
S7. Synthesizability

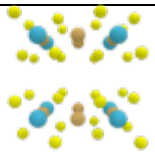
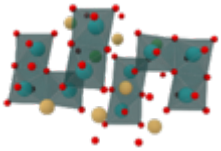
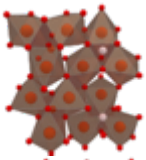
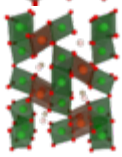
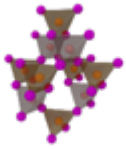
Table S3 Evidence of synthesizability for the 162 candidate compounds, including an illustration of the crystal structure, a synopsis of the synthesis method, and the corresponding literature reference. The elements in the chemical formula are ordered by increasing electronegativity.

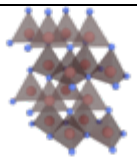
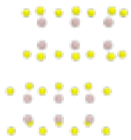
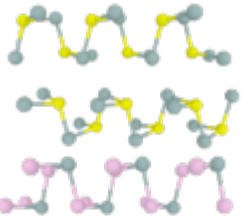
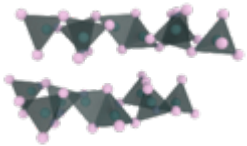
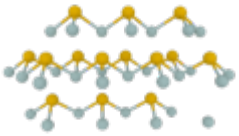
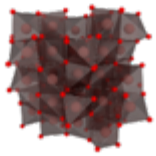
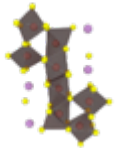
	Crystal structure	Synopsis	Reference
$AlCuO_2$		Cu_2O + Al_2O_3 + PbO at 900 °C for 48-96 hours	Ref. 1
$BaCu_2O_2$		$BaCuO_2$ ($BaCO_3$ + CuO) + Cu at 1023 K for 2 days	Ref. 2
$Ba_2Fe_2O_5$		$BaCO_3$ + α-Fe_2O_3 at 1373 K for 24 hours under nitrogen	Ref. 3
$Ba_2In_2S_5$		Ba + In + S at 1150-1250 °C in sealed ampoule	Ref. 4
Ba_2PbO_4		$BaCO_3$ + PbO_2 at 450 °C for 12 hours, then 950 °C for 12 hours in sealed ampoule, sintered in air for 24 hours at 950 °C	Ref. 5
$Ba_2SnSe_3F_2$		BaF_2 + BaS + SnSe + Se in sealed ampoule at 700 °C for 12 hours	Ref. 6
$Ba_3MnNb_2O_9$		$BaCO_3$ + MnO_2 + Nb_2O_5 at 850 °C for 20 hours, then 1350 °C for 5 days	Ref. 7
$Ba_3Zn_5In_2O_{11}$		BaO + ZnO + In_2O_3 in HNO_3 + KO_2 at 750 °C for 12 days	Ref. 8
$Ba_6Mn_5O_{16}$		$BaCO_3$ + MnO_2 in air at 1250 °C for 3 days and quenched	Ref. 9

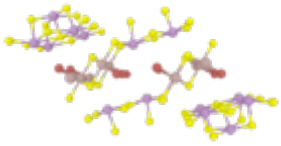
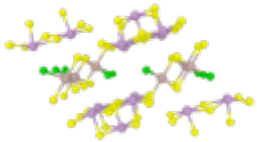
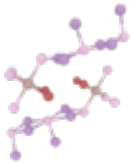
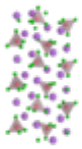
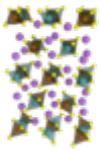
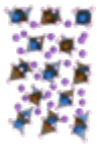
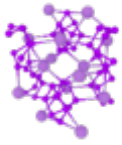
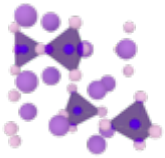
	Crystal structure	Synopsis	Reference
$Ba_6V_4S_{11}O_5$		BaS + V + V_2O_5 + S in sealed ampoule at 1198 K for 4 days	Ref. 10
$Ba_8Sb_6S_{17}$		BaS + Sb_2O_3 at 1120 K	Ref. 11
$BaAlSi_5N_7O_2$		Ba + Si_3N_4 + AlN heated to 1600 °C for 8 hours	Ref. 12
$BaCaFe_4O_8$		$BaNO_3$ + $CaCO_3$ + FeO in air at 1100 °C	Ref. 13
$BaHfN_2$		Ba_3N_2 (Ba in molten Na at 250 °C, heated to 520 °C under N_2, then 350 °C for 24 hours under vacuum) + HfN_2 in Mo foil welded, heated to 1000 °C for 5 days under Ar	Ref. 14
$BaIn_2O_4$		$BaCO_3$ + In_2O_3 at 840 °C for 12 hours	Ref. 15
BaS_2		BaS + S in sealed ampoule at 800 °C	Ref. 16
$BaSbSe_2F$		BaF_2 + Ba + Sb_2Se_3 + Se at 700 °C in sealed ampoule	Ref. 17
$BaSnS_2$		BaS + SnS at 750 °C for 2 weeks	Ref. 18
$Ca_{12}Al_{14}O_{33}$		CaO + Al_2O_3 at 453 K for 1 weeks, 1623 K for 24 hours, then 1623 K for 48 hours	Ref. 19

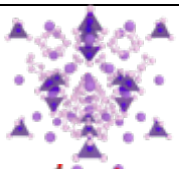
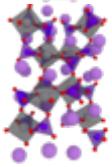
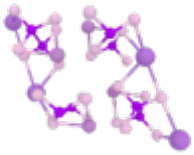
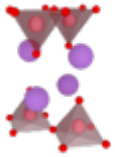
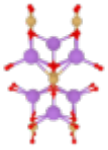
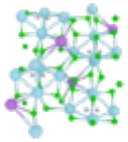
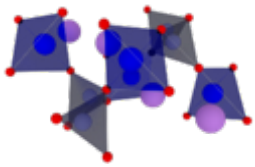
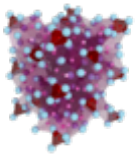
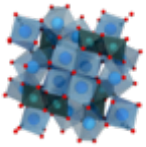
	Crystal structure	Synopsis	Reference
Ca_2CoO_3		$CaCO_3$ + Co_3O_4 ball-milled in IPA and calcined at 900 °C for 17 days	Ref. 20
Ca_2FeClO_3		$CaCl_2$ + Fe_2O_3 in $CaCl_2$ flux at 850 °C for 5 hours in Pt crucible	Ref. 21
Ca_2PbO_4		$CaCoO_3$ and PbO in 2:1 ratio at 800 °C for 72 hours	Ref. 22
Ca_3PCl_3		Ca_3P_2 + $CaCl_2$ in steel ampoules under Ar at 740 °C then 950 °C	Ref. 23
$CaFeClO_2$		$CaCl_2$ + Fe_2O_3 at 800 °C for 6 hours in Pt crucible	Ref. 21
$CaIn_2O_4$		In_2O_3 + CaO at 1400 °C for 24 hours	Ref. 24
$CaSb_{10}S_6O_{10}$		CaO + $SrCO_3$ + Sb_2S_3 + Sb_2O_3 at 100-650 °C hydrothermally	Ref. 25
$CaTaNO_2$		$CaCO_3$ + Ta_2O_5 at 900 °C in ammonia	Ref. 26
$CoPb_2WO_6$		PbO + WO_3 + CoO in sealed ampoule at 1050 K for 12 hours	Ref. 27
Cr_3BO_6		$Cr_2(SO_4)_3$-$6H_2O$ + H_3BO_3 ball-milled and fired at 680 °C for 3 days	Ref. 28

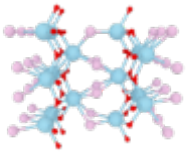
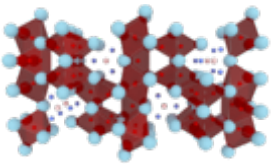
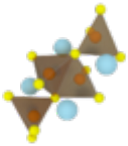
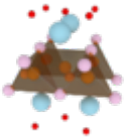
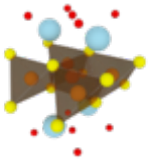
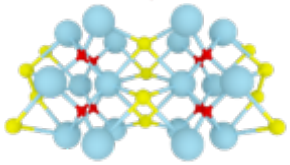
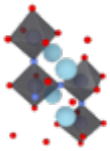
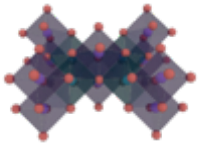
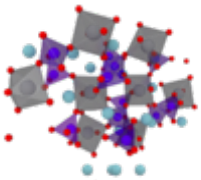
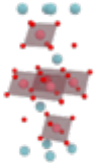
	Crystal structure	Synopsis	Reference
$CrPb_5O_8$		PbO + $Pb_2O(CrO_4)$ (CrO_3 + PbO + NaOH hydrothermally at 120 °C for 18 h) in air at 900 °C	Ref. 29
$Cs_4Ta_2S_{11}$		Cs_2S_3 (Cs + S in liquid NH3) + Ta + S in sealed ampoule at 773 K for 2 days	Ref. 30
$Cs_4Ti_3S_{14}$		Ti + S + Cs_2S_3 flux (Cs + S in NH3) heated to 873 K for 4 days	Ref. 31
$Cs_4Zr_3Se_{14}$		Zr + Se + Cs_2Se_3 (Cs+Se in liquid NH_3)	Ref. 31
$CsCuO_2$		CsO_2 + CuO under flowing oxygen at 400 °C for 6 days	Ref. 32
$CsGeI_3$		HI + H_3PO_2 + GeI_4 + CsI (colloidal)	Ref. 33
$CsLaNb_2O_7$		Cs_2CO_3 + La_2O_3 + Nb_2O_5 in 4:1:2 ratio at 1273 K in air	Ref. 34
$CsMnBr_3$		Can be synthesized colloidally or via thin film fabrication	Ref. 35
$CsMnI_3$		MnI_2 (prepared from the elements and purified by sublimation) + CsI at 380 °C for 7 days in sealed ampoule	Ref. 36
$CsSbS_2$		Hydrothermal synthesis of Cs_2S and Sb_2S_3	Ref. 37

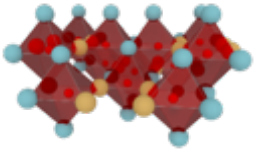
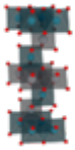
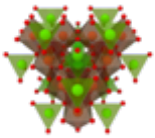
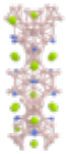
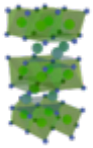
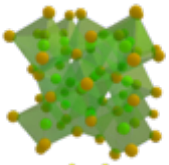
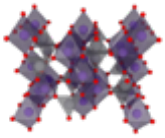
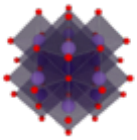
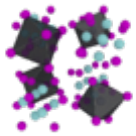
	Crystal structure	Synopsis	Reference
Cu_2WS_4		Can be synthesized colloidally	Ref. 38
Cu_3SbS_3		Cu_2S + Sb_2S_3 at 853 K in sealed quartz tube	Ref. 39
$Cu_4Mo_5O_{17}$		Cu_2O + MoO_3 in sealed ampoule	Ref. 40
CuI		Can be purchased	Ref. 41
CuP_2		Copper halide + red P + hexadecane via Schlenk technique	Ref. 42
Fe_3BO_6		Na_3BO_3 + Fe_2O_3 at 200 °C, then 1200 °C in air for 18 hours then heated in boiling water then treated with HCl	Ref. 43
$FeNi_2BO_5$		NiO + Fe_2O_3 + B_2O_3 at 1100 °C for 4 hours	Ref. 44
Ga_2TeSe_2		Ga_2Se_3 + Ga_2Te_3 at 800 K for 1 year	Ref. 45
$GaCuI_4$		CuI + GaI_3 in sealed ampoule at 573 K (slow cooling to room temp at 1 K/hour)	Ref. 46
$GaCuO_2$		Na_2CO_3 + Ga_2O_3 at 900 °C for 20 hours, then mixed with CuCl and fired at 250 °C for 48 hours under vacuum	Ref. 47

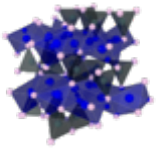
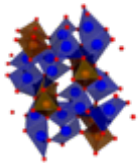
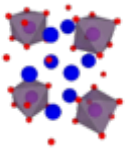
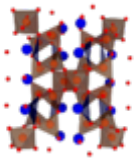
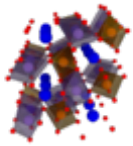
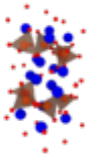
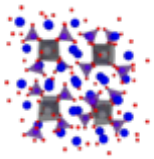
	Crystal structure	Synopsis	Reference
GaN		Can be made via thin film fabrication	Ref. 48
GaS		Can be synthesized colloidally or via thin film fabrication	Ref. 49
Ge_4Se_9		Ta + Ge + Se + RbCl in sealed ampoule at 1073 K for 96 h	Ref. 50
GeS		Can be made via thin film fabrication	Ref. 51
GeSe		Can be synthesized colloidally	Ref. 49
$GeSe_2$		Ge + Se at 1173 K for 48 hours in sealed quartz tube	Ref. 52
GeTe		Ge + Te in sealed ampoule at 1000 °C for 24 hours	Ref. 53
In_2O_3		Can be purchased	Ref. 54
$In_4Bi_2S_9$		Bi + In + S + I via CVT with temperature gradient of 680-600 °C	Ref. 55
InBr		In + $InBr_3$	Ref. 49

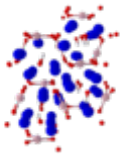
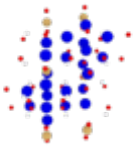
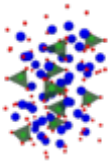
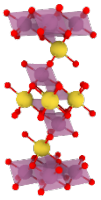
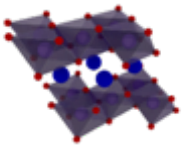
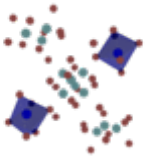
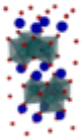
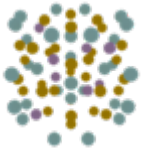
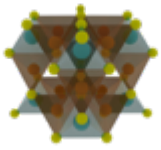
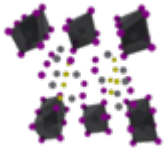
	Crystal structure	Synopsis	Reference
InI		In + I via sublimation with 200 °C to 100 °C gradient	Ref. 49
$InSb_2S_4Br$		In + $SbBr_3$ + Sb + S at 450 °C in sealed ampoule	Ref. 56
$InSb_2S_4Cl$		In + $SbCl_3$ + Sb + S at 450 °C in sealed ampoule	Ref. 56
$InSb_2Se_4Br$		In + $SbBr_3$ + Sb + Se in sealed quartz ampoule	Ref. 56
K_2CoCl_4		KCl + $CoCl_2$ melted, annealed in sealed quartz tube at 400 °C for 1 week (phase change after several months)	Ref. 57
K_2NbCuS_4		K_2S_3 + Cu +Nb + S at 623 K for 6 days	Ref. 58
$K_2TaCuSe_4$		K_2Se_5 + Ta + Cu + Se in sealed ampoule at 950 °C	Ref. 59
$K_3LaP_2Se_8$		Se + K_2Se_4 + P + La in sealed ampoule at 725 °C for 150 hours	Ref. 60
K_3P_{11}		K + P in sealed ampoule at 380 °C for 12 h, 470 °C for 86 hours	Ref. 61
K_3PSe_{16}		K_2Se_3 (K + Se in liquid NH_3) + P_2Se_5 (P + Se in ampoule at 450 °C for 24 hours) + Se + 1 mL acetonitrile heated to 110 °C for 24 hours	Ref. 62

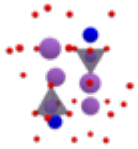
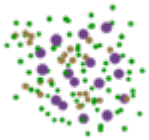
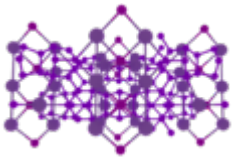
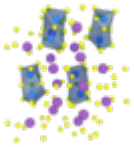
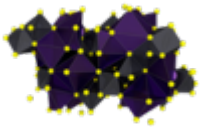
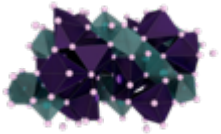
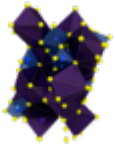
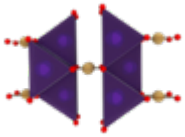
	Crystal structure	Synopsis	Reference
K_3PSe_4		P + Se + K_2Se_2 in sealed ampoule at 500 °C for 150 hours	Ref. 63
$K_3VP_2O_8$		K_2CO_3 + $H(NH_4)_2PO_4$ + V_2O_5 at 673 K in air + V in sealed ampoule at 972 K for 1 week	Ref. 64
$K_4P_{21}I$		K + P + I in sealed ampoule at 373 K for 3 days	Ref. 65
$KBiP_2Se_6$		K_2Se + Bi + P_2Se_5 + Se in sealed quartz tube at 200 °C	Ref. 66
$KCoO_2$		K_2CO_3 + Co_3O_4 at 1133-1203 K in air	Ref. 67
$KCuO_2$		KO_2 + CuO under flowing oxygen at 400 °C for 6 days	Ref. 32
$KLa_5C_2Cl_{10}$		$LaCl_3$ + K + La + C in sealed Nb ampoule at 700-900 °C	Ref. 68
$KNaZnO_2$		Na_2ZnO_2 + K_2ZnO_2 in sealed Ag cylinder under Ar at 500-600 °C for 7-14 days	Ref. 69
$La_{10}Se_{14}O$		La + Se + SeO_2 + CsCl in sealed ampoule at 800 °C for 4 days	Ref. 70
$La_4Mo_2O_{11}$		La_2O_3 + MoO_3 + Mo in sealed Mo crucible at 1980 K for 48 hours	Ref. 71

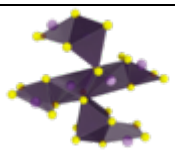
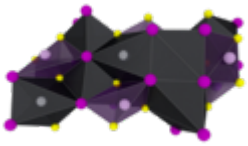
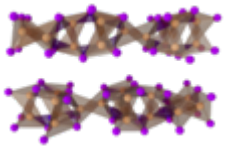
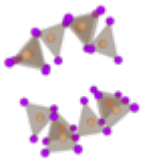
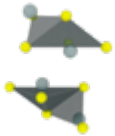
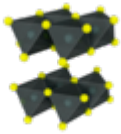
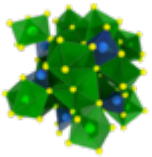
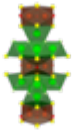
	Crystal structure	Synopsis	Reference
$La_4Se_3O_4$		La + Se + SeO_2 in sealed quartz tube heated to 750 °C for 168 hours	Ref. 72
$La_6BN_3O_6$		Li_3BN_2 + Li_3N + LaOCl at 950 °C	Ref. 73
$LaCuS_2$		$La_2Cu_2O_5$ (La_2O_3 + Cu_2O) + S	Ref. 74
LaCuSeO		La_2O_3 + La_2Se_3 (La + Se at 300 °C) + Cu + Se at 800 °C	Ref. 75
LaCuSO		La_2O_3 + La_2S_3 + Cu_2S at 800 °C	Ref. 75
LaSO		S + K_2S + La_2O_3 at 923 K under Ar	Ref. 76
$LaTiNO_2$		La_2O_3 + TiO_2 in air at 1050 °C for 24 hours, 1310 °C in air for 24 hours, ammonia flow at 950 °C for 20 hours	Ref. 77
Li_2MnBr_4		LiBr + $MnBr_2$ in sealed quartz ampoule at 1100 °C	Ref. 78
$Li_3V_2P_3O_{12}$		V_2O_5 + LiOH-H_2O + $NH_4H_2PO_4$ + C at 800 °C for 24 h	Ref. 79
$LiCoO_2$		CoO + Li_2CO_3	Ref. 80

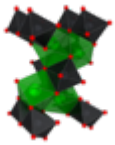
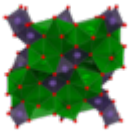
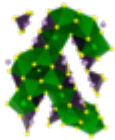
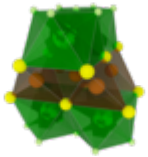
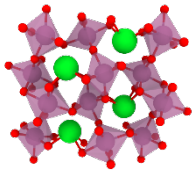
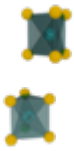
	Crystal structure	Synopsis	Reference
$LiCuO$		Li_2O + Cu_2O at 1073 K for 6 hours in sealed quartz ampoule	Ref. 81
$LiVO_2$		Li_2CO_3 + V_2O_5 under Ar/H_2 at 625 °C for 14 hours, 750 °C for 4 hours	Ref. 82
$MgFe_2O_4$		MgO + Fe_2O_3 in air at 900 °C	Ref. 83
MgB_9N		Mg + B in a BN crucible in a W container at 1873 K under Ar for 1 hours, then under vacuum for 15 minutes at 1023 K	Ref. 84
$MgMoN_2$		NaN_3 + Mo + Mg in autoclave at 700 °C for 10 hours	Ref. 85
$MgTe_2$		Mg + Te in sealed ampoule at 670 K for 15 hours, 770 K for 15 hours	Ref. 86
$MnGa_2S_4$		Mn + Ga + S in sealed ampoule at 600 °C for 2 days, 900 °C for 2 days and quenched	Ref. 87
$Mn_3V_2O_8$		MnO + V_2O_5 + MoO_3 in Pt crucible at 1110 °C for 1 hours	Ref. 88
MnO		Can be purchased	Ref. 89
Mo_6PbI_{14}		PbI_2 + MoI2 at 600 °C for 1 week	Ref. 90

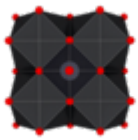
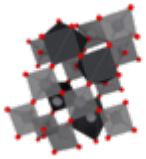
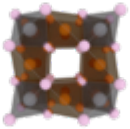
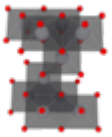
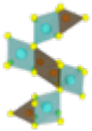
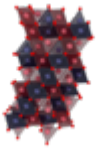
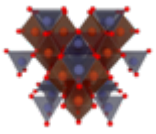
	Crystal structure	Synopsis	Reference
MoS_2		Can be synthesized colloidally	Ref. 91
$MoSe_2$		Can be synthesized colloidally	Ref. 92
$Na_2Sn_2Se_5$		Na_2Se + Sn + Se at 450 °C in sealed quartz ampoule	Ref. 93
Na_2TeO_4		NaOH + $Te(OH)_6$ in hydrothermal furnace at 580 °C	Ref. 94
Na_3BiO_4		Na_2O_2 + Bi_2O_3 at 600 °C for 12 hours (or 700 °C for 30h)	Ref. 95
$Na_3Fe_5O_9$		Na_2CO_3 + Fe_2O_3 at 1100 °C	Ref. 96
$Na_3Mn_4Te_2O_{12}$		MnO_2 + $Te(OH)_6$ in 1 M NaOH in autoclave at 648 K for 5 days	Ref. 97
Na_3WN_3		W_2N (WO_3 + NH_3 at 700 °C for 11 hours) + Na under NH_3 flow at 350 °C, then 500 °C for 8 hours, then 600 °C for 8 then 500 °C for 8 hours	Ref. 98
$Na_4Fe_2O_5$		Na_2O_2 + Fe_2O_3 at 600 °C for 6 days	Ref. 99
$Na_4VP_2O_9$		$Na_4P_2O_7$ + VO_2 in sealed ampoule at 700 °C for 3 days	Ref. 100

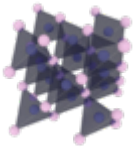
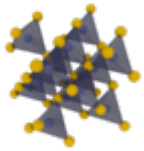
	Crystal structure	Synopsis	Reference
Na_5CoHO_4		Na_2O + CdO + NaOH + Co under Ar at 600 °C for 21 days	Ref. 101
$Na_5CuH_2O_4$		Na_2O (Na + NaOH) + NaOH + Cu_2O in Ni/Ag container sealed ampoule at 600 °C for 5 days	Ref. 102
Na_5NiO_4		Na_2O + $NaNiO_2$ at 550 °C for 2 days	Ref. 103
$NaInO_2$		Na_2CO_3 + In_2O_3 at 1100 °C for 48 hours	Ref. 104
$NaMnO_2$		Na_2CO_3 + MnO	Ref. 105
$NaMo_6Br_{13}$		$MoBr_2$ + NaBr in sealed ampoule at 700 °C	Ref. 106
$NaNbO_2$		Na_2O + NbO + NbO_2 at 700 °C for 3 days	Ref. 107
$Nb_3Sb_2Te_5$		Nb + Sb + Te in sealed quartz ampoule at 600 °C for 2 weeks	Ref. 108
$NbCu_3S_4$		Cu + Nb + S + I via CVT with temperature gradient of 1123-1053 K for 120 hours	Ref. 109
$Pb_5S_2I_6$		Pb + S + I at 600 °C	Ref. 110

	Crystal structure	Synopsis	Reference
PbO		Can be purchased	Ref. 111
Rb_2MnCl_4		RbCl + $MnCl_2$ in sealed ampoule until molten, then cooled slowly	Ref. 112
Rb_2NaMnO_4		Na_2O + Rb_2O + Mn + CdO in Ag crucibles sealed in ampoule heated to 523 K for 14 days	Ref. 113
$Rb_4Cu_5Cl_9$		RbCl + CuCl at 220 °C, then 160 °C for 96 hours	Ref. 114
$Rb_4P_{21}I$		Rb + P + I in sealed ampoule at 373 K for 3 days	Ref. 115
$Rb_4Ta_2S_{11}$		Rb_2S_3 (Rb_2S_3 (Rb + S in liquid NH_3) + Ta + S in sealed ampoule at 773 K for 6 days	Ref. 30
$Rb_4Ti_3S_{14}$		Ti + S + Rb_2S_3 flux (Rb + S in NH_3) heated to 873 K for 4 days	Ref. 31
$Rb_4Zr_3Se_{14}$		Zr + Se + Rb_2Se_3 (Rb + Se in liquid ammonia) in sealed ampoule at 873 K for 4 days	Ref. 31
$Rb_6Ta_4S_{25}$		Rb_2S_3 (Rb + S in liquid ammonia under Ar) + Ta + S in sealed ampoule at 723 K for 5 days	Ref. 116
$RbCuO_2$		RbO_2 + CuO under flowing oxygen at 400 °C for 6 days	Ref. 32

	Crystal structure	Synopsis	Reference
Sb_2S_3		Can be purchased	Ref. 117
$SbPb_2S_2I_3$		PbS + Sb_2S_3 + I in CVT with sealed quartz tube at 600 °C for 12 days	Ref. 118
SiP		Si + P + Sn in 500 °C in sealed ampoule for 36 h, then 1150 °C for 10 hours	Ref. 119
SiP_2		Si + P in sealed quartz tube at 1200 °C	Ref. 120
SnS		Can be synthesized colloidally	Ref. 121
SnS_2		Can be synthesized colloidally	Ref. 122
$SrCu_2O_2$		SrO + Cu_2O at 800 °C	Ref. 123
$Sr_{17}Ta_{10}S_{42}$		$SrCO_3$ + Ta_2O_5 + S in sealed ampoule at 700 °C for 48 hours	Ref. 124
$Sr_2Fe_2S_2OF_2$		SrF_2 + SrO + Fe + S in sealed ampoule at 800 °C for 12 hours	Ref. 125
Sr_2FeBrO_3		Fe_2O_3 + $SrCO_3$ + $SrBr_2$ at 850 °C in air for 4 days	Ref. 126

	Crystal structure	Synopsis	Reference
Sr_2FeClO_3		Fe_2O_3 + $SrCO_3$ + $SrCl_2$ at 850 °C in air for 4 days	Ref. 126
Sr_2FeO_3F		SrF_2 + SrO_2 + Fe at 3 GPa and 1300 °C	Ref. 127
Sr_2PbO_4		PbO + $SrCO_3$ at 1073 K in air	Ref. 128
$Sr_2SnSe_3F_2$		SrF_2 + SrS + SnSe + Se in sealed ampoule at 700 °C for 12 hours	Ref. 6
$Sr_4Mn_3O_{10}$		SrO + $Sr(NO_3)_2$ + Mn_2O_3 in sealed ampoule at 1100 °C for 12 hours	Ref. 129
$Sr_6Sb_6S_{17}$		Sr + Sb + S in sealed ampoule at 800 °C for 5 days	Ref. 130
SrCuSeF		$SrSe_2$ + SrF + Cu_2Se in sealed ampoule at 500 °C for 6 hours	Ref. 131
SrCuSF		SrF_2 + SrS ($SrSO_4$ under H_2 at 1100 °C for 15 hours) + Cu_2S in sealed ampoule 500 °C for 6 hours	Ref. 131
$SrIn_2O_4$		Solid state reaction of SrO + In_2O_3 at 1200 °C	Ref. 132
Te_2Mo		Can be synthesized colloidally	Ref. 133

	Crystal structure	Synopsis	Reference
$TiPbO_3$		PbO + TiO_2 at 900 °C	Ref. 134
$V_5(PbO_6)_2$		PbV_2O_7 (PbO + V_2O_5 at 600 °C for 5 d in air) + V_2O_3 + V_2O_5 in sealed ampoule at 730 °C for 3 days	Ref. 135
VCu_3Se_4		V + Cu + Se in sealed quartz tube at 600 °C for 6 weeks	Ref. 49
VO		V + V_2O_5 in vacuum at 1000 °C	Ref. 136
WS_2		Can be made via thin film fabrication	Ref. 137
WSe_2		Can be synthesized colloidally	Ref. 137
$YCuS_2$		Y + Cu + S in sealed ampoule at 1420 K for 4 hours	Ref. 138
$ZnCo_2O_4$		ZnO + Co_2O_3	Ref. 49
$ZnFe_2O_4$		ZnO + Fe_2O_3 at 800 °C, also can be made via flux	Ref. 139
$ZnGeP_2$		Zn + Ge + P in Bi flux in sealed ampoule	Ref. 140

	Crystal structure	Synopsis	Reference
ZnP_2		Phosphorus vapor passed over Zn in sealed quartz system	Ref. 141
ZnSe		Can be synthesized colloidally	Ref. 49
ZnTe		Can be synthesized colloidally	Ref. 142

S8. Analysis of electrochemical stability

The computational Pourbaix diagrams (Fig. S7 and Fig. S8) of the seven tested compounds are evaluated using the pymatgen (Python Materials Genomics) package [143]. The energies of the aqueous ions are corrected to reproduce the experimental dissolution energies of the reference solids as derived by Persson and coworkers [144]. All of the Pourbaix diagrams are generated by setting the ion concentrations to 10^{-6} M at 25 °C. The electrochemical (meta)stability of each target compound is evaluated by computing its free energy difference with respect to the most stable phase in each of the Pourbaix domains [145]. The energy differences for all the synthesized compounds are summarized in the bar chart in Fig. S10 by setting the pH to 1.5 and 7 that corresponds to the two test conditions. The potential is chosen to be the flat-band potential using the geometric mean of Mulliken electronegativity. In addition, preliminary XRD analyses were performed to validate the computationally predicted electrochemical stability (Fig. S9). We found a good correlation between the predicted and experimental data. Most of the compounds exhibit a low 'driving force' for decomposition (<0.5 eV/atom) [144-145]. Expectedly, the synthesized compounds are found to be more stable under neutral electrochemical conditions [condition (*ii*)] compared to acidic testing conditions [condition (*i*)].

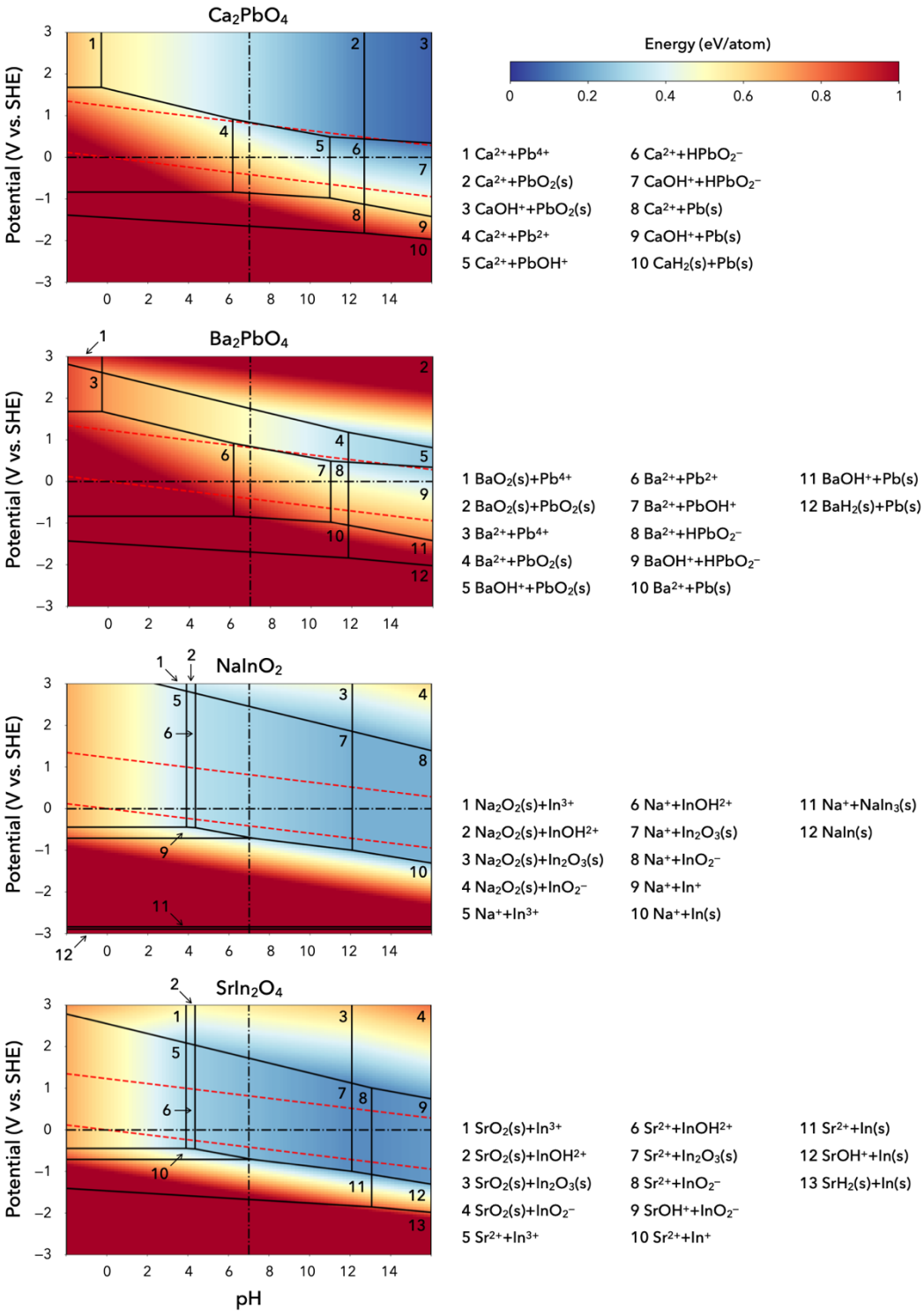


Figure S7 Computed Pourbaix diagrams of Ca_2PbO_4, Ba_2PbO_4, $NaInO_2$, and $SrIn_2O_4$. The heatmap visualizes the electrochemical stability of each compound with respect to the most stable Pourbaix phases. All of the stable Pourbaix domains are labeled.

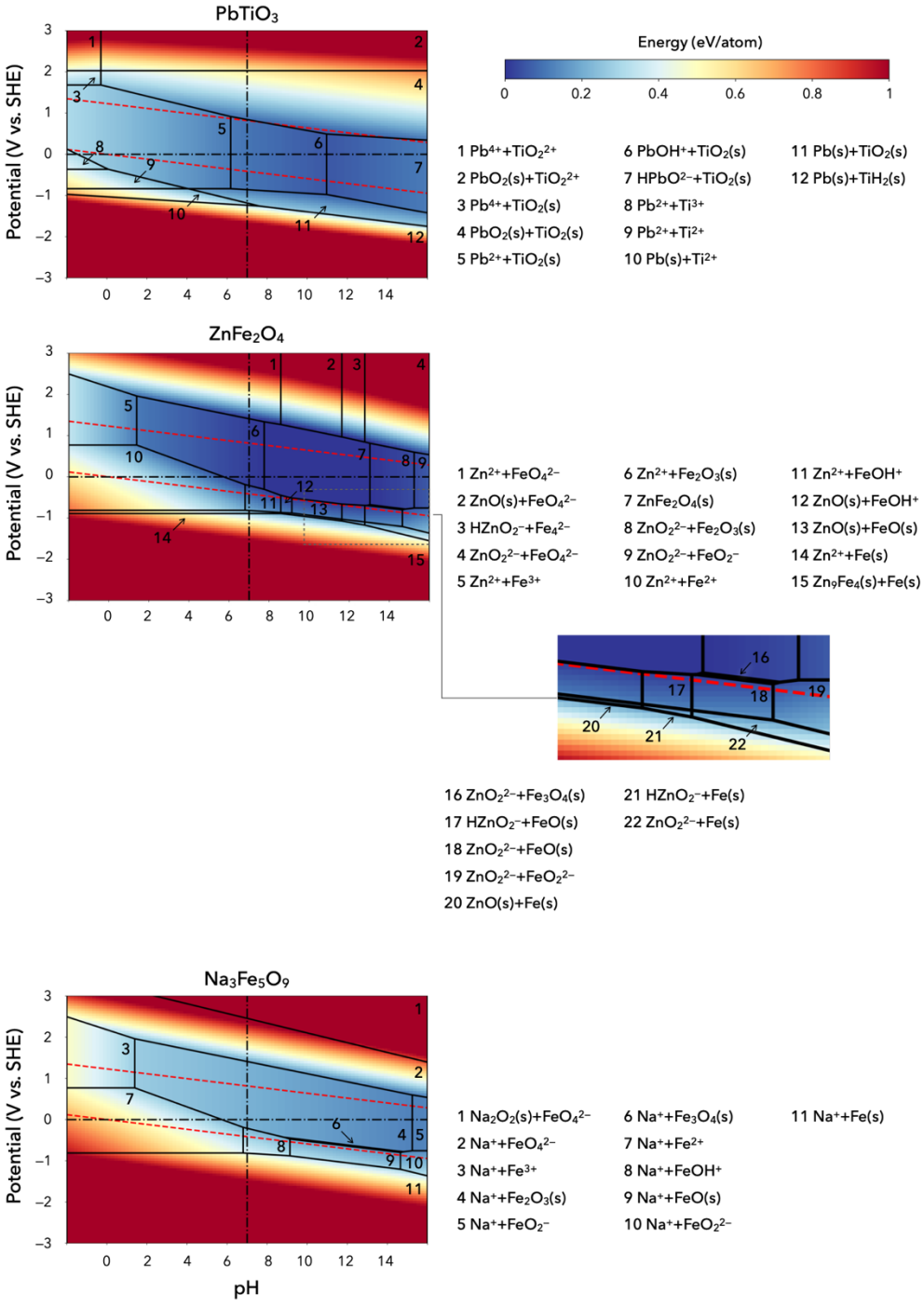


Figure S8 Computed Pourbaix diagrams of $PbTiO_3$, $ZnFe_2O_4$, and $Na_3Fe_5O_9$. The heatmap visualizes the electrochemical stability of each compound with respect to the most stable Pourbaix phases. All of the stable Pourbaix domains are labeled.

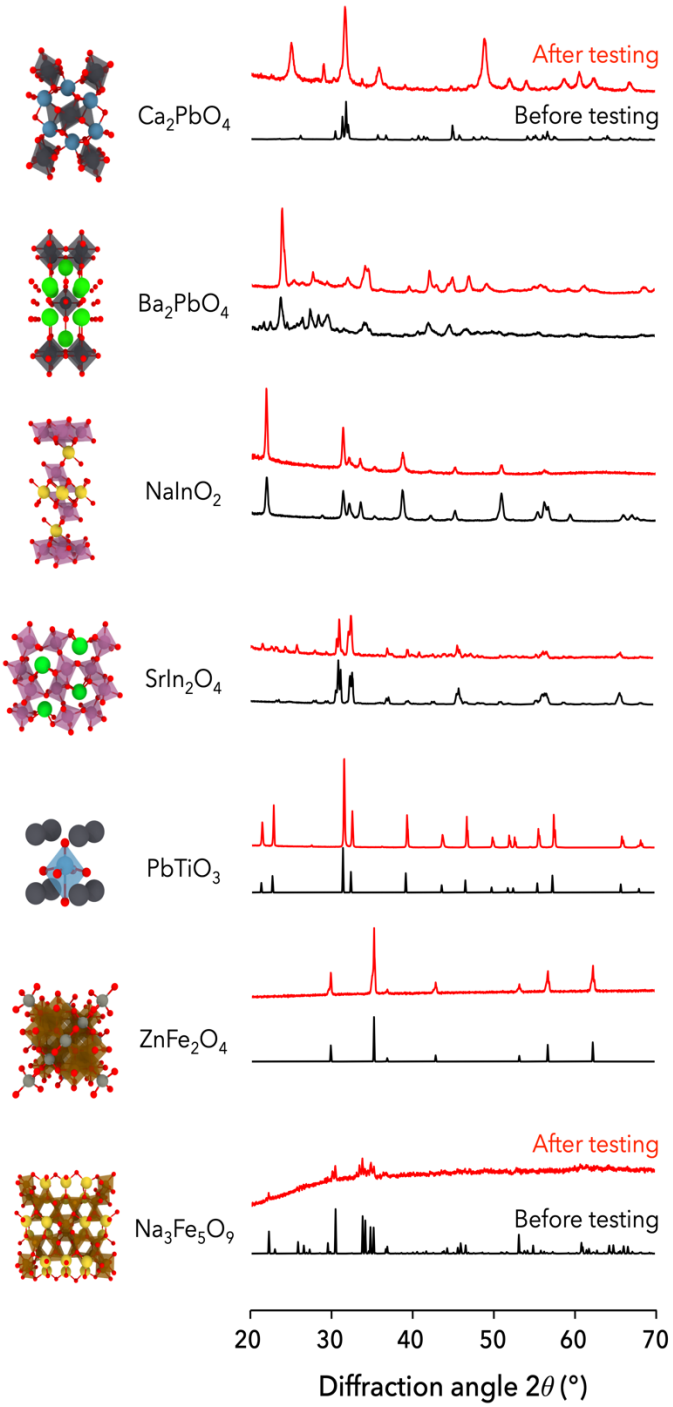


Figure S9 X-ray diffraction of the synthesized compounds before and after testing under photocatalytic conditions. Except for $Na_3Fe_5O_9$ (whose XRD pattern shows a significant background signal, while preserving the main peaks) and Ba_2PbO_4 (which corrodes in humid atmosphere) most candidates show minor changes in the XRD patterns, indicating their potential stabilities in aqueous media.

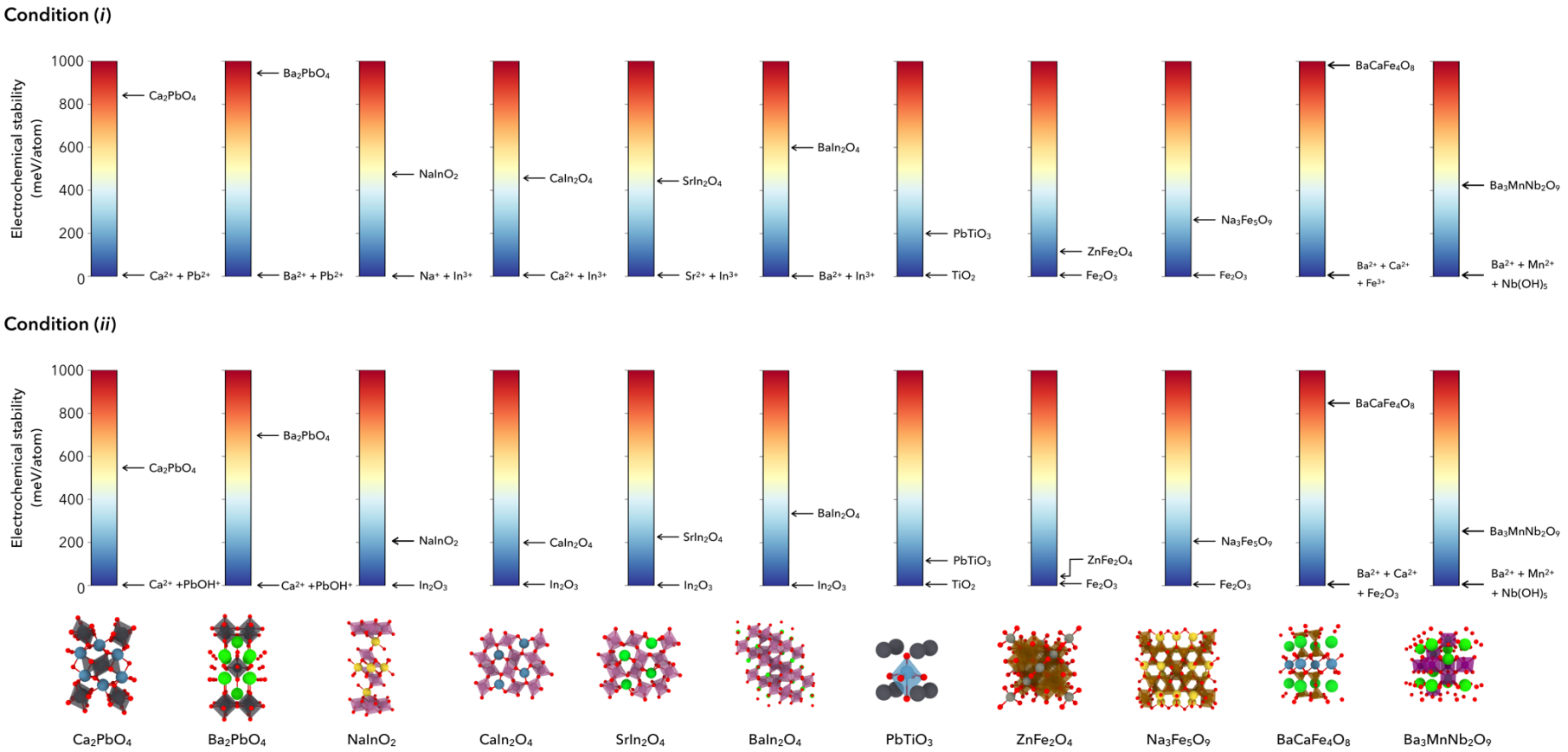


Figure S10 Predicted wlectrochemical stability energy of the synthesized compounds in aqueous solution under condition (*i*) (pH = 1.5) and condition (*ii*) (pH = 7).

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