Supporting Information

Interpretable learning of voltage for electrode design of multivalent metal-ion batteries

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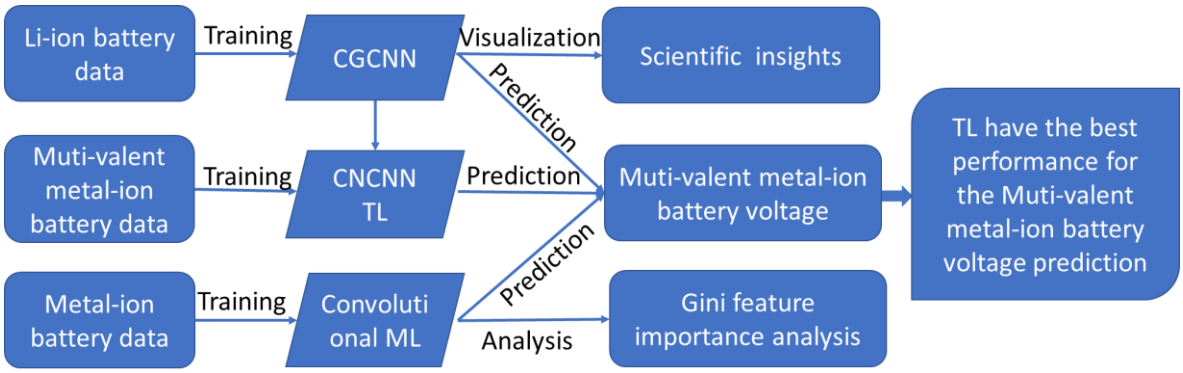
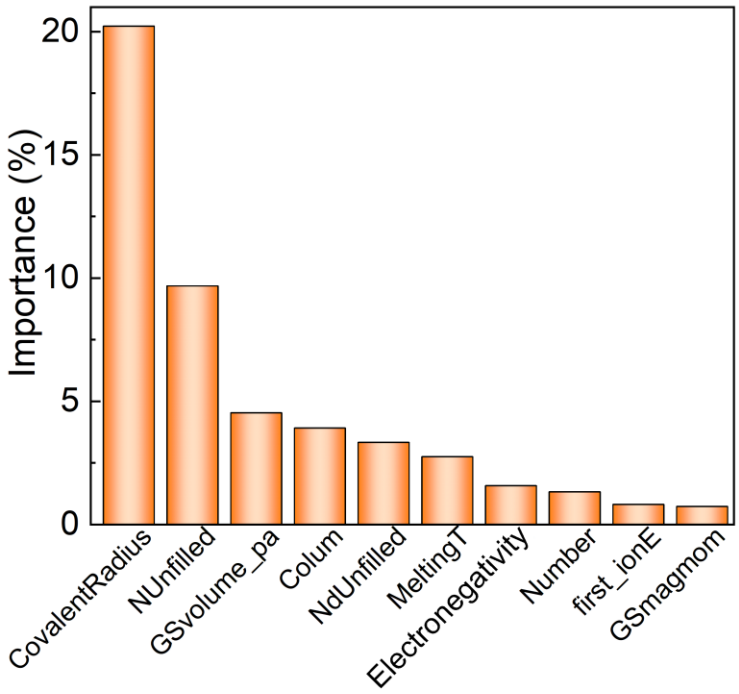
Supplementary Table 1. The dataset size of each metal-ion battery.

Ion	Li	Ca	Mg	Zn	Al	Na	K	Rb	Cs	Y
Total number	2291	484	393	385	149	328	125	50	39	157
Used number	2190	471	387	378	149	287	125	50	39	157

All data are extracted from Materials Project (MP) database through the application programming interface (API) Pymatgen. Here, the outliners for Li-, Ca-, Mg-, Zn-, and Na-ion batteries are removed, but not for others with very small data sizes. Furthermore, the extreme values of voltages are excluded in the training data set.



Supplementary Figure 1. An overview of the hierarchy structure of different models. The CGCNN model is firstly trained on the data set of Li-ion battery electrode voltages for the LIB electrode voltage prediction and model visualization and explanation. The TL model is trained based on the pre-trained CGCNN model with multivalent MIB data sets and is used for the prediction of multivalent MIB electrode voltages. For comparation with the convolutional ML models (SVR and KRR), the pre-trained CGCNN model, which is called Li-model, is also used for directly predicting the MIB electrode voltages. The convolutional ML model of RFR is also used for Gini feature importance analysis.



Supplementary Figure 2. Gini feature importance analysis for the random forest regression (RFR) model.

The RFR model uses 273 features which are the same as the SVR and KRR models used in this work. It is found that the covalent radius of the element in a crystal may significantly affect the crystal voltage with the highest Gini feature importance of 20%.

The Elemental properties in this plot are taken from The Materials Agnostic Platform for Informatics and Exploration (Magpie) and are explained as follow:

CovalentRadius: Covalent radius of atoms.

NUnfilled: The NUnfilled for one element orbital means the number of electrons in the orbital subtracted from the total number of electrons allowed in that orbital. Here the NUnfilled means the total number of all unfilled orbitals of an atom. Fully unoccupied orbitals are counted as 0.

GSvolume_pa: Specific volume at the ground state of 0 K.

Colum: Column number of an atom in the elemental periodic table.

NdUnifilled: The number of electrons in *d*-orbitals subtracted from the total number of electrons allowed in *d* orbital.

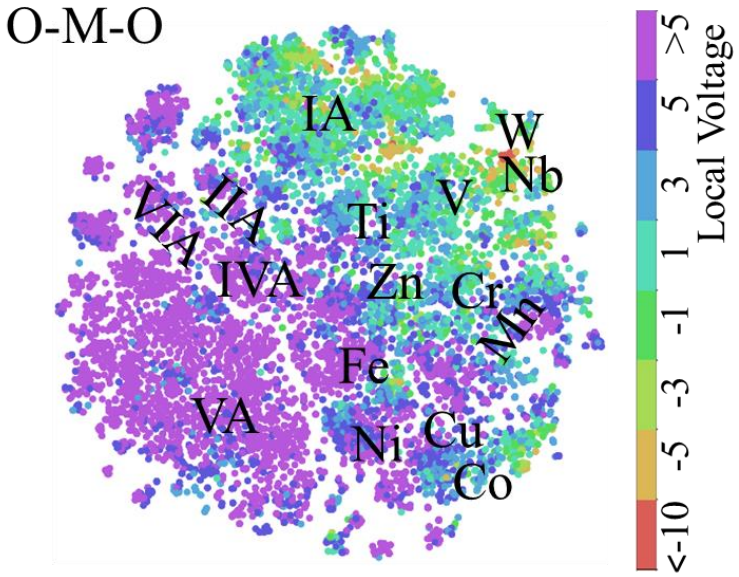
MeltingT: Melting temperature

Electronegativity: Electronegativity of an atom

Number: Atomic number of the atom in the elemental periodic table.

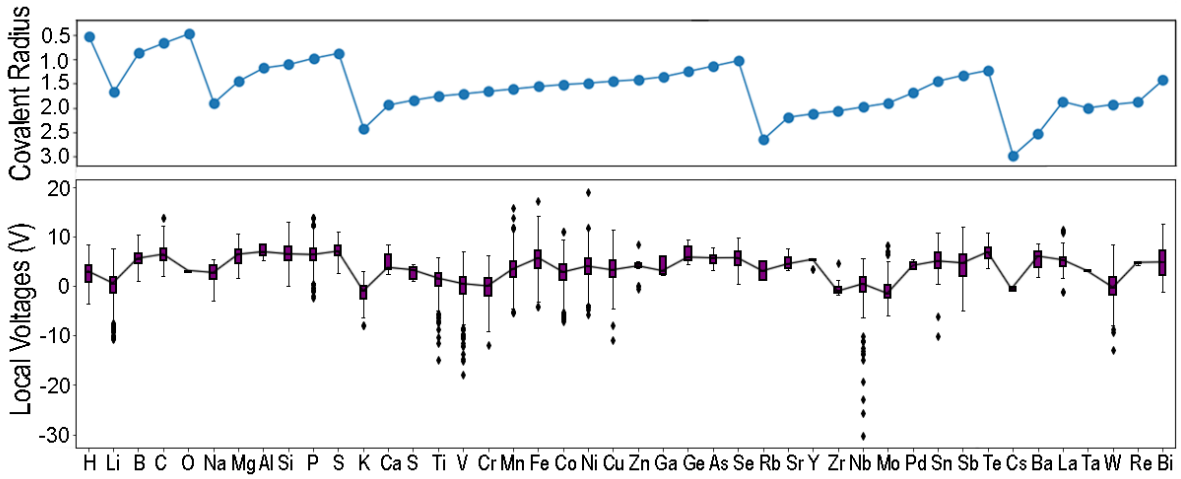
First_ionE: The first ionization energy.

GAmagmom: Magnetic moment (per atom) at the ground state of 0 K.



Supplementary Figure 3. t-SNE analysis of the local oxygen coordination environments. The points are labelled according to the type of the centre atoms in the coordination environments. The colours are coded with the learned local voltages.

Supplementary Figure 3 shows that oxygen environments can be approximately grouped into three large groups. The first group only includes the elements of group IA, which perform a low voltage in the oxygen coordination environment. The second group contains most of the main group elements which perform a high voltage. Most of the transition metal elements form the third group with various voltages.



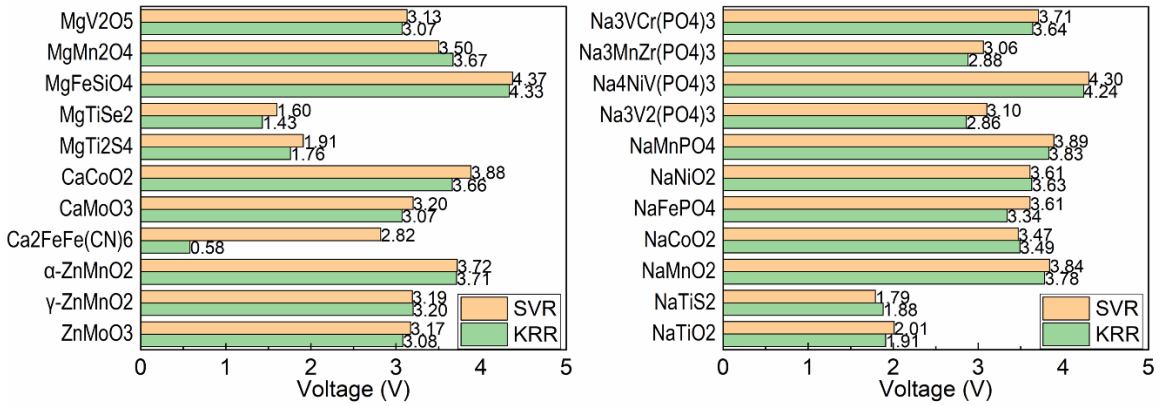
Supplementary Figure 4. Local voltages of elements in the oxygen coordination environment and the elemental covalent radius as a function of atomic number.

Supplementary Figure 4 shows the change of the local voltage in the oxygen coordination environment as a function of atomic number. The negative local voltage has a similar trend to the covalent radius of elements. The element with a higher (lower) covalent radius tends to have a lower (higher) local energy. This indicates that the voltage of a crystal is highly correlated with the covalent radius of the elements in the crystal.

Supplementary Table 2. MAEs of the Li-model and transfer learning model for predicting electrode voltages of different metal-ion batteries.

MAE (V)	Li	Mg	Ca	Zn	Al	Na	K
Li-model	0.32	1.08	0.68	2.14	1.63	0.68	0.81
Transfer learning	N. A.	0.45	0.40	0.47	0.60	0.51	0.66

It is worth noting that our Li-model (a DL model trained on LIB data sets) can be used directly for other monovalent Na- and K-ion batteries with acceptable accuracies because of the similarity between monovalent Li-, Na-, and K-ion batteries. However, for multivalent Mg-, Ca-, Zn-, and Al-ion batteries, the accuracy of prediction can be greatly increased by the transfer learning technique.



Supplementary Figure 5. Comparing the voltages of some electrodes predicted by support vector regression (SVR) and Kernel Ridge Regression (KRR) models.

Supplementary Figure 5 shows that SVR and KRR models predict similar voltages for both the monovalent and multivalent metal-ion batteries.

Supplementary Note: Details about average voltage calculation with DFT

The open-cell voltage for an intercalation electrode is defined as the chemical potential difference between the intercalation compound (μ_{Li}^{IC}) and the metallic lithium (μ_{Li}^{0}),

$$V = -\frac{\mu_{Li}^{IC} - \mu_{Li}^{0}}{zF} \quad (1)$$

where *z* is the charge that is transferred, and *F* is the Faraday constant. The lithium chemical potential is the change of the free energy of the electrode material with lithium content[1,2]. Integrating Equation (1) over a finite amount of reaction gives the average voltage as function of the free energy change of the combined anode/cathode reaction,

$$\bar{V} = -\frac{\Delta G}{zF} \quad (2)$$

Here, $\Delta G = \Delta E + P\Delta V - T\Delta S$, where ΔE is the internal energy change, P is the pressure, ΔV is the volume change, T is the temperature, and ΔS is the entropy difference of the system. However, $P\Delta V \approx 10^{-5}$ eV and $T\Delta S \approx 25$ meV at room temperature[3]. Therefore, by neglecting those two terms, we can calculate the voltage (*V*) by only considering the internal energy change. Then,

$$\bar{V} \approx -\frac{\Delta E}{zF} \quad (3)$$

Take a lithium transition-metal oxide intercalation cathode with composition $LiMO_2$ as an example. The cell discharge reaction should be

$$Li_{x1}MO_2 + (x_2 - x_1)Li \xrightarrow{\text{discharge}} Li_{x2}MO_2 \quad (x_2 > x_1)$$

The average voltage can thus be computed as

$$\bar{V} \approx -\frac{E[Li_{x2}MO_2] - E[Li_{x1}MO_2] - (x_2 - x_1)E[Li]}{(x_2 - x_1)F} \quad (x_2 > x_1) \quad (4)$$

where the internal energies of the lithiated and delithiated phases, $E[Li_{x2}MO_2]$ and $E[Li_{x1}MO_2]$, and of metallic (body-centered cubic) lithium, $E[Li]$, can be obtained from first principles.

The average interaction voltage in Materials Project is defined by the above Equations (1-4). Taking $Li_xFe_9CoO_{20}$ (ID: mp-1177006_Li) in Materials Project as an example, the voltages under 3 different lithiation states from $Li_4Fe_9CoO_{20}$ to $Li_6Fe_9CoO_{20}$, from $Li_6Fe_9CoO_{20}$ to $Li_8Fe_9CoO_{20}$, and from $Li_8Fe_9CoO_{20}$ to $Li_{10}Fe_9CoO_{20}$ are calculated with the voltage of 4.78, 4.22, and 3.97 V, respectively. In this work, the average voltage of 4.29 V between the fully charged and fully discharged stage in Materials Project is used for the electrode material of $Li_xFe_9CoO_{20}$.

Supplementary Table 3. Predicted electrode voltages for Al-ion batteries.

All materials in this table have been used as electrodes for Mg-, Ca-, and Zn-ion batteries, and we here predict their electrode voltage for Al-ion batteries.

	entry_id	formula	working_ion	pred_voltage
1	mp-568610	Bi	Al	-0.73
2	mp-23152	Bi	Al	-0.70
3	mp-569358	Bi	Al	-0.54
4	mp-567597	Bi	Al	-0.39
5	mp-542633	GdCo2	Al	-0.39
6	mvc-11235	BiN	Al	-0.36
7	mp-1008728	Ni	Al	-0.33
8	mp-1039305	MgBi	Al	-0.22
9	mp-23	Ni	Al	-0.21
10	mp-1056004	Mo	Al	-0.13
11	mp-8634	Mn	Al	-0.07
12	mvc-15478	CoN	Al	-0.06
13	mp-1383	UCo2	Al	-0.06
14	mp-929	ZrCo2	Al	0.02
15	mp-8632	V	Al	0.05
16	mvc-14421	BaCa(CoN2)2	Al	0.11
17	mvc-13841	CuN	Al	0.14
18	mvc-11274	CaCoN2	Al	0.20
19	mp-8636	Nb	Al	0.21
20	mp-7162	Sn	Al	0.23
21	mp-1343	NdNi2	Al	0.23
22	mvc-11162	NiN	Al	0.25
23	mvc-14553	FeN	Al	0.26
24	mp-25648	WO2	Al	0.28
25	mp-7564	Nb3Te4	Al	0.29
26	mp-1094371	MgTi2	Al	0.30
27	mp-589	TbFe2	Al	0.31
28	mp-1226796	Ce2ZnSb4	Al	0.32
29	mp-89	Cr	Al	0.33
30	mp-21021	Mo3Se4	Al	0.35
31	mp-6985	Ti	Al	0.38
32	mvc-10945	Ca2VN3	Al	0.40
33	mp-2250	ZrNi2	Al	0.42
34	mvc-2846	W5O7	Al	0.42
35	mp-1718	ZrFe2	Al	0.43
36	mvc-14842	BaCa3(CuN2)2	Al	0.44
37	mp-971669	FeSb3	Al	0.48
38	mp-21050	UFe2	Al	0.48
39	mvc-11104	Ca2CrN3	Al	0.50
40	mp-1096950	Fe	Al	0.50
41	mvc-11231	SbN	Al	0.51

42	mp-1097924	MgSb	Al	0.51
43	mp-1191566	Zn6Sb5	Al	0.52
44	mvc-934	W2O3	Al	0.53
45	mp-11503	MnZn	Al	0.53
46	mvc-2118	WO2	Al	0.55
47	mp-1179605	Sb	Al	0.56
48	mvc-15882	Mo2O5	Al	0.57
49	mp-133	Sb	Al	0.58
50	mp-1008753	Ti2Al	Al	0.59
51	mp-1046939	BaTl(WO3)2	Al	0.63
52	mp-561	Nb3Se4	Al	0.65
53	mp-1147769	Cu2GeS4	Al	0.67
54	mvc-13041	Ca11(MnN5)2	Al	0.68
55	mp-1046584	Ba2Tl2W3O10	Al	0.68
56	mvc-11164	Ca11(FeN5)2	Al	0.70
57	mvc-157	Mg(WO2)4	Al	0.71
58	mp-102	Co	Al	0.72
59	mp-1039074	MgBi	Al	0.72
60	mp-1045898	V9O13	Al	0.72
61	mp-637219	Mo4O5	Al	0.73
62	mvc-5928	WO2	Al	0.75
63	mp-1014230	TiZn	Al	0.77
64	mp-715584	MoO3	Al	0.78
65	mp-12627	Nb3S4	Al	0.81
66	mp-1041454	Ba(WO2)4	Al	0.81
67	mp-7761	Sb	Al	0.82
68	mp-714883	MoO2	Al	0.82
69	mp-21855	VCu3Se4	Al	0.83
70	mp-2164	Mo3S4	Al	0.84
71	mp-1043388	V2O3	Al	0.86
72	mp-1044751	Pr(WO3)2	Al	0.87
73	mvc-5033	MoWO6	Al	0.87
74	mp-1047152	IrWO6	Al	0.92
75	mp-1047232	WO2	Al	0.93
76	mp-21594	Ca9Zn4Sb9	Al	0.93
77	mp-1009730	Ca2Sn	Al	0.94
78	mvc-14086	Ca5(MnN3)2	Al	0.94
79	mp-1116820	MoWO6	Al	0.95
80	mp-1042291	WO2	Al	0.96
81	mp-1094669	MgSn	Al	0.96
82	mp-1190582	Mg6NbH16	Al	0.97
83	mp-1041282	WO2	Al	0.97
84	mp-19529	W18O49	Al	0.98
85	mvc-15895	W2O5	Al	0.99
86	mp-1094565	MgSb	Al	1.00
87	mp-1040834	WO2	Al	1.00

88	mvc-6377	MoO2	Al	1.00
89	mp-1047616	WO2	Al	1.02
90	mvc-13677	MoO2	Al	1.03
91	mvc-13180	CrSe2	Al	1.04
92	mp-714969	MoO2	Al	1.06
93	mvc-11744	Ca(TiS2)4	Al	1.06
94	mp-1191852	Mg6TiH16	Al	1.08
95	mp-1191096	Mg6VH16	Al	1.08
96	mp-2156	TiS2	Al	1.08
97	mp-1048022	W4O9	Al	1.09
98	mp-9027	TiS2	Al	1.09
99	mp-1046039	V5O7	Al	1.13
100	mp-1041271	BaV4O8	Al	1.14
101	mp-1046025	Mg(MoO2)4	Al	1.14
102	mp-1044267	TiV(PO4)3	Al	1.14
103	mp-754767	Fe3(SnS4)2	Al	1.15
104	mvc-13133	Cu2SnSe4	Al	1.17
105	mp-547271	ReO3	Al	1.18
106	mvc-12231	MgV4O8	Al	1.18
107	mp-1041295	Ho(WO3)2	Al	1.20
108	mp-1047618	VO2	Al	1.21
109	mp-1040961	P2W2O9	Al	1.21
110	mp-1047430	Ba(SbO2)4	Al	1.21
111	mp-1046654	Sr2CrSO3	Al	1.22
112	mvc-11754	V2S5	Al	1.26
113	mp-1094572	Mg2Sb	Al	1.26
114	mp-1047798	CuMoO4	Al	1.28
115	mp-1041997	MoO2	Al	1.29
116	mp-656884	Ni9O10	Al	1.33
117	mp-1013526	VS2	Al	1.33
118	mp-117	Sn	Al	1.33
119	mvc-13140	Cu2GeSe4	Al	1.34
120	mvc-13032	Ba2Cu2HgO6	Al	1.34
121	mp-1047927	V3P3O13	Al	1.34
122	mp-1044451	PrTi2O6	Al	1.35
123	mp-1047842	Ba(MoO2)4	Al	1.36
124	mp-1047421	BaTi4O8	Al	1.36
125	mvc-11852	Ba2CaTl2(CuO3)4	Al	1.36
126	mp-1048593	Ca(TiS2)2	Al	1.36
127	mvc-12771	MgV2O6	Al	1.38
128	mp-1046501	Ba2Tl2Co3O10	Al	1.42
129	mvc-12466	TiO2	Al	1.43
130	mvc-15991	Mo3O8	Al	1.44
131	mvc-13223	VO2	Al	1.44
132	mp-714944	VO2	Al	1.45
133	mvc-12789	ScMo3O8	Al	1.45

134	mvc-15237	Ba4CaCu6(HgO8)2	Al	1.47
135	mvc-93	Ca(MnS2)4	Al	1.49
136	mvc-11834	BaTlCuO4	Al	1.49
137	mp-1047621	MoO2	Al	1.49
138	mvc-12077	VO2	Al	1.49
139	mp-777836	Li14Co13O28	Al	1.49
140	mp-1046652	Sr2FeSO3	Al	1.50
141	mp-608555	Cs2SnCl6	Al	1.50
142	mvc-15011	Ca3Nd4Nb6(FeO14)2	Al	1.50
143	mp-1041993	MoO2	Al	1.51
144	mvc-12918	Sb5S3O5	Al	1.52
145	mvc-12176	CaTi4O8	Al	1.52
146	mvc-11086	V2O5	Al	1.53
147	mp-1041288	BaCr4O8	Al	1.53
148	mvc-5310	VO2	Al	1.53
149	mp-1044744	Pr(MoO3)2	Al	1.53
150	mvc-5548	VO2	Al	1.54
151	mp-1046608	Sr3Co2S2O5	Al	1.54
152	mp-1043919	LaFeWO6	Al	1.54
153	mp-510748	V2O5	Al	1.54
154	mvc-12866	SbO2	Al	1.54
155	mp-1042928	Fe2(MoO4)3	Al	1.55
156	mp-1047280	Ba(SnO2)4	Al	1.56
157	mvc-11089	VO2	Al	1.57
158	mvc-14991	SrCuSO	Al	1.58
159	mp-1009813	SiSn	Al	1.59
160	mvc-14769	CrS2	Al	1.60
161	mvc-12039	Fe5O7	Al	1.62
162	mp-1040910	VO2	Al	1.62
163	mvc-12595	Mn2ZnO4	Al	1.62
164	mp-715479	Mo3O8	Al	1.62
165	mp-1044382	TiCr(PO4)3	Al	1.63
166	mvc-13047	Ba2CaTl2(CuO3)4	Al	1.63
167	mp-1041394	La2WO6	Al	1.64
168	mp-1041198	Ho(MoO3)2	Al	1.65
169	mp-1045759	Ti5O7	Al	1.65
170	mvc-15230	MgV2O6	Al	1.67
171	mvc-11885	Ba4CaTl4(Cu3O10)2	Al	1.67
172	mp-1041213	P4W3O14	Al	1.67
173	mvc-10959	VBiO5	Al	1.67
174	mp-1046632	Sr2CoSO3	Al	1.67
175	mp-1047075	MoO2	Al	1.67
176	mp-1041196	Ti3P3O13	Al	1.67
177	mp-1045643	Ti9O13	Al	1.68
178	mvc-14243	CaCoO3	Al	1.68
179	mp-1045293	Ca(SbO3)2	Al	1.68

180	mvc-12321	CaSb2S5	Al	1.68
181	mp-1044002	LaTaFeO6	Al	1.68
182	mp-1046793	Ti2O3	Al	1.69
183	mvc-12227	Mn3Nb2O9	Al	1.70
184	mp-1042978	W3O8	Al	1.71
185	mvc-14257	Mo3O8	Al	1.71
186	mp-1094498	Mg5Ti	Al	1.72
187	mp-1227103	CaNb4O14	Al	1.72
188	mp-1045734	MgV2O6	Al	1.73
189	mvc-12205	Fe9O13	Al	1.73
190	mvc-15486	W3O8	Al	1.74
191	mvc-14274	ZnCr4O8	Al	1.74
192	mp-1044162	PWO5	Al	1.74
193	mp-1047986	MgTi4O8	Al	1.75
194	mvc-11828	Ca2CuIrO6	Al	1.75
195	mvc-12005	Fe2O3	Al	1.75
196	mp-1042860	Fe2(WO4)3	Al	1.75
197	mvc-12286	Ca2Nb2CoO9	Al	1.76
198	mvc-13329	Sr9Zn2(CuO7)2	Al	1.76
199	mvc-12581	MgCr4O8	Al	1.79
200	mp-1221467	MoO4	Al	1.79
201	mp-1216303	VPO5	Al	1.81
202	mvc-14832	Ca2CuRhO6	Al	1.82
203	mp-1044853	TiO2	Al	1.82
204	mp-1045634	Zn(FeO2)4	Al	1.83
205	mp-1046050	Cr5O7	Al	1.83
206	mp-1040930	Mo2P2O9	Al	1.84
207	mp-769727	Li3(NiO2)4	Al	1.84
208	mp-1046617	Sr2MnSO3	Al	1.84
209	mp-1046082	Co5O7	Al	1.85
210	mp-1043379	Cr2O3	Al	1.85
211	mp-1045826	Cr9O13	Al	1.85
212	mp-1048765	Mg(SbO3)2	Al	1.86
213	mvc-11686	SnO2	Al	1.86
214	mp-1043966	LaVFeO6	Al	1.87
215	mvc-10909	Ca3Ta2Mn2O12	Al	1.87
216	mp-1046932	BaTl(NiO3)2	Al	1.87
217	mp-1225007	Fe5O8	Al	1.87
218	mvc-12889	Ca3Co2(TeO6)2	Al	1.87
219	mp-1147673	Cu3O4	Al	1.88
220	mvc-11423	TiO2	Al	1.88
221	mp-1042407	CuW2O7	Al	1.89
222	mvc-13694	La2MoO6	Al	1.89
223	mp-1042994	Cr3(FeO6)2	Al	1.90
224	mvc-2949	SbO2	Al	1.90
225	mp-1041961	CrO2	Al	1.90

226	mp-1046591	Ba2Tl2Ni3O10	Al	1.91
227	mvc-11183	SrCuBiO4	Al	1.91
228	mp-1043944	LaFeMoO6	Al	1.92
229	mp-1047920	Mo3P3O13	Al	1.93
230	mp-1046066	Mn5O7	Al	1.94
231	mp-1046942	Nb2MoO8	Al	1.94
232	mp-1047047	Ti3(P2O7)2	Al	1.94
233	mvc-12404	TiO2	Al	1.94
234	mp-1047643	CrO2	Al	1.95
235	mvc-15048	MnNb2ZnO8	Al	1.96
236	mvc-11373	CaMnWO6	Al	1.96
237	mvc-12278	CaV4(CuO7)2	Al	1.97
238	mp-25620	V2O5	Al	1.98
239	mvc-13124	Mg3V2(BiO6)2	Al	1.98
240	mp-1043995	LaFeSbO6	Al	1.98
241	mp-1043875	Ni2O3	Al	1.98
242	mvc-12134	Mn2Nb2O9	Al	1.98
243	mp-1045304	Zn(SbO3)2	Al	1.98
244	mp-1041165	Ti2Be3(SiO4)3	Al	1.99
245	mvc-7566	Ta2CoO7	Al	1.99
246	mp-756655	TiO2	Al	1.99
247	mp-25433	TiO2	Al	1.99
248	mp-1043418	Co2O3	Al	2.00
249	mp-1214031	CaC4	Al	2.00
250	mvc-13146	HoV2O6	Al	2.01
251	mvc-5774	CrWO6	Al	2.01
252	mp-1044716	SbO2	Al	2.01
253	mp-1047639	CoO2	Al	2.02
254	mp-25593	NiO2	Al	2.03
255	mp-1047121	CrO2	Al	2.03
256	mp-25547	MnO2	Al	2.03
257	mp-1143521	Si2WO6	Al	2.03
258	mp-1044440	Pr(SbO3)2	Al	2.04
259	mp-25476	CoO2	Al	2.04
260	mp-1044164	MoPO5	Al	2.04
261	mvc-11564	CoO2	Al	2.04
262	mp-1043389	NiP2WO9	Al	2.04
263	mvc-11947	CaV2O6	Al	2.05
264	mvc-4408	Ge3(MoO6)2	Al	2.06
265	mp-1043363	Mn2O3	Al	2.06
266	mp-1018795	Mg2Sn	Al	2.07
267	mvc-12611	CaCr4O8	Al	2.07
268	mvc-14106	CaVBiO6	Al	2.07
269	mvc-12603	Mg(FeO2)2	Al	2.08
270	mvc-10923	Ca(FeO2)2	Al	2.08
271	mvc-12916	V6Zn(FeO6)4	Al	2.08

272	mp-1045833	Mn9O13	Al	2.08
273	mp-1045896	Ni9O13	Al	2.08
274	mp-1041292	Ba(CoO2)4	Al	2.09
275	mp-1045698	V2ZnO6	Al	2.10
276	mvc-13330	V3O7	Al	2.11
277	mp-1041225	HoCr2O6	Al	2.11
278	mp-1003641	MgMn2O4	Al	2.11
279	mvc-5626	MoAsO5	Al	2.11
280	mvc-15363	SnO2	Al	2.11
281	mvc-14931	MnO2	Al	2.11
282	mvc-5659	SnO2	Al	2.12
283	mvc-10908	Ca3Mn2(SbO6)2	Al	2.12
284	mp-1045581	Zn(CoO2)4	Al	2.12
285	mp-1044028	LaFeBiO6	Al	2.12
286	mvc-10961	V4O9	Al	2.12
287	mp-1046949	Nb2WO8	Al	2.13
288	mp-1044227	BiWO5	Al	2.13
289	mp-1045694	Cu9O13	Al	2.13
290	mvc-13175	Ta2MnZnO8	Al	2.14
291	mvc-5000	CrWO6	Al	2.14
292	mvc-12760	CaNiWO6	Al	2.14
293	mvc-4401	Ge3(WO6)2	Al	2.14
294	mp-774537	Ti2(PO4)3	Al	2.15
295	mp-1044492	Pr(SnO3)2	Al	2.15
296	mvc-12122	VCuO4	Al	2.15
297	mp-1046815	BaTl(CoO3)2	Al	2.15
298	mp-1042388	BiSbO5	Al	2.15
299	mp-1044987	Zn(NiO2)4	Al	2.17
300	mvc-4364	BiO2	Al	2.18
301	mp-1047762	NiO2	Al	2.18
302	mp-1046820	Cu2O3	Al	2.18
303	mp-714929	CrO2	Al	2.18
304	mp-1047300	SbO2	Al	2.19
305	mp-1040783	Ho(SbO3)2	Al	2.19
306	mp-568806	C	Al	2.19
307	mp-1043235	V(GeO3)2	Al	2.19
308	mp-1039182	Mg2Bi	Al	2.19
309	mvc-9896	SnO2	Al	2.20
310	mvc-11007	CaFeMoO6	Al	2.20
311	mvc-2263	Co9O13	Al	2.20
312	mvc-14981	Ca3Fe2(SbO6)2	Al	2.20
313	mvc-5485	CrO2	Al	2.21
314	mp-775220	V(GeO3)2	Al	2.21
315	mvc-14096	Cu3(GeO3)4	Al	2.21
316	mvc-5171	TiO2	Al	2.21
317	mvc-14986	CaNiWO6	Al	2.22

318	mvc-5627	NiO2	Al	2.22
319	mvc-10916	CaFeWO6	Al	2.23
320	mp-1046357	Ta2WO8	Al	2.23
321	mvc-14970	Ti4(FeO4)3	Al	2.24
322	mp-656880	Y2Mn2S2O5	Al	2.24
323	mvc-14468	MgV6(FeO6)4	Al	2.24
324	mp-1046180	SrTi(PO4)2	Al	2.25
325	mvc-15207	Ta2Bi2O9	Al	2.25
326	mvc-5220	BiO2	Al	2.25
327	mvc-12565	Mg(CoO2)4	Al	2.26
328	mvc-11950	CaNd2Ti2Mn2O12	Al	2.26
329	mvc-11561	MnO2	Al	2.26
330	mvc-11334	Ca3(CuO3)2	Al	2.26
331	mp-1047467	Ba(BiO2)4	Al	2.26
332	mvc-11541	FeO2	Al	2.26
333	mvc-14237	CaCoWO6	Al	2.26
334	mvc-12570	Mg(NiO2)4	Al	2.27
335	mp-1143551	Si3(WO6)2	Al	2.27
336	mp-1094189	Mg5Sn	Al	2.27
337	mp-19395	MnO2	Al	2.27
338	mvc-13117	CaLa2Ti2Cr2O12	Al	2.27
339	mvc-9006	LaCrFeO6	Al	2.28
340	mp-1047381	SnO2	Al	2.29
341	mp-1040967	CrO2	Al	2.29
342	mvc-5592	P2WO7	Al	2.29
343	mvc-13203	CoO2	Al	2.29
344	mvc-5236	SnO2	Al	2.29
345	mp-19326	MnO2	Al	2.30
346	mp-1046192	Sn5(TeO6)3	Al	2.30
347	mp-1041470	CrCuO4	Al	2.31
348	mp-1043495	TiNiP2O9	Al	2.31
349	mvc-11309	Cr2S5	Al	2.32
350	mvc-5295	CrO2	Al	2.32
351	mvc-11632	VBiO5	Al	2.33
352	mp-1044910	VPO4	Al	2.33
353	mvc-12283	MnO2	Al	2.33
354	mvc-13123	CaFeReO6	Al	2.33
355	mp-1041066	MnO2	Al	2.33
356	mp-1041312	BaMn4O8	Al	2.34
357	mvc-14589	CrO2	Al	2.34
358	mp-25519	FeO2	Al	2.35
359	mvc-6353	MnO2	Al	2.35
360	mp-1043195	V(GeO3)2	Al	2.36
361	mp-1043472	NiMoP2O9	Al	2.36
362	mvc-14984	Ca3Co2(RhO6)2	Al	2.36
363	mvc-15035	Ca3Ga2(FeO5)2	Al	2.36

364	mvc-11942	CaTi2Fe2(PO4)6	Al	2.36
365	mvc-11930	Ca3Mn2(GaO5)2	Al	2.37
366	mp-33009	MnO2	Al	2.37
367	mp-1044829	Sn2P2O9	Al	2.37
368	mp-540258	Ti(PO3)4	Al	2.38
369	mp-1044823	Ti2P2O9	Al	2.38
370	mp-1041231	Sn3P3O13	Al	2.39
371	mvc-14929	CaLa2Ti2Mn2O12	Al	2.40
372	mvc-12304	V2P2O9	Al	2.40
373	mvc-4715	TiO2	Al	2.40
374	mp-1046527	Cr5(TeO6)3	Al	2.42
375	mvc-11581	CrO2	Al	2.43
376	mp-1041980	NiO2	Al	2.43
377	mvc-14940	Ti(BiO3)2	Al	2.43
378	mvc-5444	MnO2	Al	2.43
379	mvc-15145	Zn3Cu10(TeO6)6	Al	2.43
380	mvc-10874	Ba(FeO2)4	Al	2.44
381	mvc-10912	CaMnIrO6	Al	2.45
382	mp-1046448	SrCr(PO4)2	Al	2.45
383	mvc-14254	Ca3Fe2(RhO6)2	Al	2.45
384	mp-32416	V3(P2O7)2	Al	2.45
385	mvc-12901	NiO2	Al	2.46
386	mvc-13028	CaCu2F8	Al	2.46
387	mvc-12905	FeO2	Al	2.47
388	mvc-13126	Ca5Sc2(CoO6)2	Al	2.47
389	mvc-13490	Bi2O5	Al	2.47
390	mp-1190609	VO2	Al	2.47
391	mp-1046509	Mn5(TeO6)3	Al	2.48
392	mvc-14949	Ti(BiO3)2	Al	2.49
393	mp-1046486	Ta2CrO8	Al	2.49
394	mp-543057	MnO2	Al	2.50
395	mp-1043013	Cr3O8	Al	2.50
396	mvc-11380	V2CoO7	Al	2.51
397	mvc-12170	CoO2	Al	2.51
398	mp-782692	Mn7O12	Al	2.51
399	mp-1047386	BiO2	Al	2.52
400	mp-1041256	NiO2	Al	2.52
401	mp-1118309	TiO2	Al	2.52
402	mvc-12204	FeO2	Al	2.53
403	mp-25301	Ti(SiO3)2	Al	2.54
404	mvc-11924	Mg3Bi2(AsO6)2	Al	2.55
405	mvc-10906	Ca2MnNiO6	Al	2.56
406	mp-1042873	Sn(GeO3)2	Al	2.56
407	mvc-5346	TiP2O7	Al	2.56
408	mvc-12807	CaMnFeO5	Al	2.57
409	mp-1047059	CrIrO6	Al	2.57

410	mp-773884	Bi19O30	Al	2.58
411	mvc-15204	Ta2Bi2O9	Al	2.59
412	mp-1046704	VPO5	Al	2.59
413	mp-644514	MnO2	Al	2.59
414	mvc-12050	NiO2	Al	2.60
415	mp-1117519	Cr2O5	Al	2.60
416	mvc-5816	CoO2	Al	2.63
417	mp-1047829	Ba(NiO2)4	Al	2.64
418	mvc-13572	Mn2Be3(SiO4)3	Al	2.64
419	mp-1143651	Si3(MoO6)2	Al	2.67
420	mp-1040999	CuTeO4	Al	2.68
421	mp-1046421	SrV(PO4)2	Al	2.69
422	mp-1047285	FeO2	Al	2.69
423	mp-1044472	Pr(BiO3)2	Al	2.69
424	mp-1044170	CrPO5	Al	2.70
425	mvc-11996	Zn3Bi2(PO6)2	Al	2.70
426	mp-1046640	Ni5(TeO6)3	Al	2.70
427	mp-1040838	Ho(BiO3)2	Al	2.71
428	mp-1046184	SrSn(PO4)2	Al	2.71
429	mvc-15135	FeO2	Al	2.71
430	mvc-12806	Mg3Bi2(PO6)2	Al	2.71
431	mvc-8434	Cr(GeO3)2	Al	2.71
432	mvc-15502	Cr2O5	Al	2.71
433	mp-540180	Cr3(P2O7)2	Al	2.71
434	mp-998866	C	Al	2.72
435	mvc-13145	Zn3Cu2(AsO4)4	Al	2.73
436	mp-1041443	Cr4O9	Al	2.74
437	mvc-11916	Ca2La5Mn7NiO24	Al	2.74
438	mp-1048779	Mg(BiO3)2	Al	2.75
439	mvc-5644	VAsO5	Al	2.75
440	mp-1043760	Si4WO10	Al	2.75
441	mp-1045326	Zn(BiO3)2	Al	2.76
442	mp-770908	CoO2	Al	2.76
443	mvc-11093	MnO2	Al	2.76
444	mvc-5268	SbAsO5	Al	2.76
445	mp-1116784	CoO2	Al	2.77
446	mp-1043651	BiSbO5	Al	2.77
447	mvc-14167	WF5	Al	2.79
448	mvc-11781	CaTi2F10	Al	2.79
449	mvc-14980	CaMn2O5	Al	2.80
450	mp-1043556	SbPO5	Al	2.80
451	mp-25633	V(SiO3)2	Al	2.81
452	mp-1046490	SrFe(PO4)2	Al	2.81
453	mp-540486	Fe3(P2O7)2	Al	2.83
454	mp-1043403	Si4SnO10	Al	2.83
455	mvc-13059	Ca3Cu6(AsO4)8	Al	2.83

456	mvc-13696	NiO2	Al	2.84
457	mp-1046454	SrCo(PO4)2	Al	2.84
458	mvc-12739	CaCu2(GeO3)4	Al	2.85
459	mvc-11633	VPO5	Al	2.86
460	mp-1044639	Fe(GeO3)2	Al	2.86
461	mp-1045327	Ca(BiO3)2	Al	2.86
462	mp-1046983	Nb2CrO8	Al	2.86
463	mp-1043373	Bi2O5	Al	2.86
464	mvc-14253	Ca3Mn2O7	Al	2.87
465	mp-1043501	Fe(GeO3)2	Al	2.87
466	mvc-11848	CaBiAsO6	Al	2.88
467	mvc-12133	V2Zn3(P2O9)2	Al	2.88
468	mvc-8359	Cr(GeO3)2	Al	2.88
469	mvc-12125	FeO2	Al	2.88
470	mp-1043652	V(Si2O5)2	Al	2.91
471	mp-1042757	CrAs2O7	Al	2.91
472	mp-1042045	NiO2	Al	2.93
473	mvc-5466	CoO2	Al	2.93
474	mp-1221542	MnO2	Al	2.93
475	mvc-12038	Mn4(SiO3)5	Al	2.94
476	mvc-12282	MgV2(SiO4)3	Al	2.94
477	mp-1048924	FePO4	Al	2.95
478	mvc-3816	WF5	Al	2.95
479	mvc-14217	MoF5	Al	2.97
480	mp-1048029	Ni3P3O13	Al	2.98
481	mvc-12280	Ba2CaV2(P2O9)2	Al	2.98
482	mvc-13642	VF4	Al	2.98
483	mp-1044247	NiSnP2O9	Al	3.00
484	mp-769642	Fe(CO3)2	Al	3.00
485	mp-1044399	Mn(GeO3)2	Al	3.00
486	mp-767563	P4WO12	Al	3.01
487	mvc-10979	CaCu2(GeO3)4	Al	3.02
488	mvc-13181	FeO2	Al	3.03
489	mp-1044873	Bi2P2O9	Al	3.03
490	mp-1045817	Ba2CuMo2F14	Al	3.04
491	mvc-14396	PrMn2O6	Al	3.06
492	mp-775128	Fe3Sb(PO4)6	Al	3.06
493	mp-1043461	NiSbP2O9	Al	3.06
494	mvc-13706	Cr3O8	Al	3.06
495	mvc-12174	CrPO4	Al	3.07
496	mvc-12302	Ca8Cr(PO4)7	Al	3.07
497	mvc-11883	Ca3Cu6(PO4)8	Al	3.08
498	mvc-3781	MoF5	Al	3.09
499	mp-1043383	Mn(GeO3)2	Al	3.09
500	mvc-5643	CrAsO5	Al	3.09
501	mvc-12312	VNiP2O9	Al	3.09

502	mvc-13172	Ba4CaV4Cu2F28	Al	3.09
503	mvc-12063	FeO2	Al	3.11
504	mp-851050	Ca9Co(PO4)7	Al	3.11
505	mp-1042331	Mn(SiO3)2	Al	3.12
506	mvc-15457	La2CrO6	Al	3.12
507	mp-1221093	NaCaFe(SiO3)4	Al	3.12
508	mp-1041261	Bi3P3O13	Al	3.13
509	mvc-10933	CaLa2Mn2(FeO6)2	Al	3.13
510	mvc-12020	CaMnSi2O7	Al	3.13
511	mp-1043406	Ti(Si2O5)2	Al	3.13
512	mvc-11862	CaCu2(As2O7)2	Al	3.14
513	mvc-15019	V2(PO4)3	Al	3.14
514	mvc-11925	MgBiPO6	Al	3.15
515	mp-1047904	Cr3P3O13	Al	3.16
516	mp-1040982	Cr2P2O9	Al	3.16
517	mp-32442	VP2O7	Al	3.17
518	mp-1043316	Ni(GeO3)2	Al	3.17
519	mp-1043444	Ni(GeO3)2	Al	3.19
520	mvc-8361	Co(GeO3)2	Al	3.21
521	mp-1043245	Co(GeO3)2	Al	3.22
522	mp-1045006	Ba2Ti2CuF14	Al	3.22
523	mvc-11375	Mg2Mn2(SiO4)3	Al	3.23
524	mp-540363	VP2O7	Al	3.24
525	mp-1041062	Fe2P2O9	Al	3.25
526	mp-25502	Cr(SiO3)2	Al	3.26
527	mvc-13536	CrF4	Al	3.27
528	mp-1142841	Cr(Si2O5)2	Al	3.29
529	mp-1042286	Co(SiO3)2	Al	3.29
530	mp-771678	NaFe2(SiO3)4	Al	3.30
531	mvc-12287	Mg2Fe2(SiO4)3	Al	3.30
532	mp-1043741	NiBiP2O9	Al	3.31
533	mvc-11865	CaCoSi2O7	Al	3.32
534	mvc-5296	BiAsO5	Al	3.32
535	mvc-12787	CaCu2(Si2O5)4	Al	3.32
536	mp-1046462	SrMn(PO4)2	Al	3.33
537	mvc-12271	Ca2Fe2(SiO4)3	Al	3.33
538	mp-1043728	Mn(Si2O5)2	Al	3.34
539	mp-25523	Fe(SiO3)2	Al	3.36
540	mvc-12258	Ca2Mn2(SiO4)3	Al	3.36
541	mp-765928	VF5	Al	3.37
542	mp-694554	Mn3(P2O7)2	Al	3.38
543	mvc-11637	Fe3P3O13	Al	3.39
544	mp-1043700	Fe(Si2O5)2	Al	3.40
545	mvc-13960	FeF4	Al	3.42
546	mp-1142713	Mn(SiO3)2	Al	3.43
547	mp-1221188	NaCa3Fe(SiO3)8	Al	3.45

548	mp-1043826	Si4NiO10	Al	3.48
549	mp-540500	Co3(P2O7)2	Al	3.48
550	mp-1044071	CrNiP2O9	Al	3.48
551	mp-1047608	Co3(AsO4)4	Al	3.49
552	mvc-14848	CaCu2(P2O7)2	Al	3.50
553	mvc-10920	CaFe2F10	Al	3.53
554	mvc-12815	Bi6P2O15	Al	3.53
555	mp-1043669	Co(Si2O5)2	Al	3.54
556	mp-673105	Cu3(P2O7)2	Al	3.55
557	mp-1117500	SnF4	Al	3.57
558	mp-1047928	Mn3P3O13	Al	3.57
559	mvc-14312	VF5	Al	3.57
560	mp-1043619	FeNiP2O9	Al	3.59
561	mp-766786	VF5	Al	3.62
562	mp-1043595	MnNiP2O9	Al	3.62
563	mp-1040954	Mn2P2O9	Al	3.62
564	mp-1044234	Ni2P2O9	Al	3.62
565	mvc-12012	Co(SiO3)2	Al	3.66
566	mp-1043572	BiPO5	Al	3.68
567	mp-32527	V(PO3)4	Al	3.68
568	mvc-12198	Fe(SiO3)2	Al	3.71
569	mvc-13125	Si2NiO6	Al	3.71
570	mvc-14697	SbF5	Al	3.72
571	mvc-13941	CoF4	Al	3.73
572	mvc-4499	Cr2(GeO4)3	Al	3.74
573	mvc-1739	Ba2CuSn2F14	Al	3.75
574	mp-765763	Cr(SO4)2	Al	3.78
575	mp-540430	CrP2O7	Al	3.78
576	mp-540321	FeP2O7	Al	3.78
577	mp-1047945	BaWF7	Al	3.83
578	mp-773979	Cr(SO4)2	Al	3.84
579	mvc-7342	Si2NiO6	Al	3.85
580	mp-32394	Ni3(P2O7)2	Al	3.85
581	mvc-6713	Ni3(AsO4)4	Al	3.85
582	mp-540267	CrP2O7	Al	3.86
583	mp-1172462	Cr2(SiO4)3	Al	3.86
584	mvc-15098	SrNi(PO4)2	Al	3.86
585	mvc-2979	MnF4	Al	3.87
586	mvc-14215	CrF5	Al	3.87
587	mvc-10914	CrP2O7	Al	3.98
588	mvc-3813	CrF5	Al	3.99
589	mvc-13241	Ba2Cr2CuF14	Al	4.00
590	mp-1047957	BaMoF7	Al	4.01
591	mp-540262	CoP2O7	Al	4.04
592	mp-687212	Cr(PO3)4	Al	4.05
593	mvc-15217	Bi3(PO5)2	Al	4.06

594	mp-694636	MnP2O7	Al	4.10
595	mvc-12753	CaMn2F10	Al	4.10
596	mp-31998	Mn(PO3)4	Al	4.14
597	mvc-15884	NiF4	Al	4.14
598	mp-32334	NiP2O7	Al	4.15
599	mvc-14958	Ba2CaCr2F14	Al	4.15
600	mvc-11142	CrF6	Al	4.16
601	mp-690058	FeP2O7	Al	4.18
602	mp-585256	Co(PO3)4	Al	4.24
603	mvc-12243	Ba2Fe2CuF14	Al	4.24
604	mvc-12100	CoP2O7	Al	4.25
605	mvc-15137	Ba2ZnFe2F14	Al	4.28
606	mvc-15798	BiF5	Al	4.34
607	mp-1041341	BaSbF7	Al	4.37
608	mp-695808	Ni(PO3)4	Al	4.38
609	mp-540273	NiP2O7	Al	4.39
610	mvc-3518	BiF5	Al	4.41
611	mp-1048114	BaCrF7	Al	4.55
612	mp-1045769	Ba2Mn2CuF14	Al	4.61
613	mp-1041349	BaBiF7	Al	4.70

Supplementary Table 4. Predicted electrode voltages for Ca-ion batteries.

The crystals have been used as electrodes for Mg-, Zn-, and Al-ion batteries, and we here predict their electrode voltage for Ca-ion batteries.

	entry_id	formula	working_ion	pred_voltage
1	mp-998866	C	Ca	-2.19
2	mp-1061123	TiAl	Ca	-0.64
3	mvc-4059	TiSiO4	Ca	-0.59
4	mp-8636	Nb	Ca	-0.23
5	mp-1094034	Ti3C2	Ca	-0.01
6	mp-80	Sb	Ca	0.32
7	mp-2649	Zr5Sb3	Ca	0.39
8	mp-1055908	Mn	Ca	0.50
9	mp-569358	Bi	Ca	0.53
10	mp-510522	Zr5Sn3	Ca	0.67
11	mp-117	Sn	Ca	0.70
12	mp-23152	Bi	Ca	0.81
13	mp-8632	V	Ca	0.83
14	mp-1065340	W	Ca	0.83
15	mp-1094371	MgTi2	Ca	0.89
16	mp-1047986	MgTi4O8	Ca	0.92
17	mp-10631	Sb	Ca	0.95
18	mp-1097924	MgSb	Ca	1.02
19	mp-6985	Ti	Ca	1.03
20	mp-1008753	Ti2Al	Ca	1.08

21	mp-568345	Fe	Ca	1.10
22	mp-1718	ZrFe2	Ca	1.10
23	mp-567597	Bi	Ca	1.11
24	mp-91	W	Ca	1.15
25	mp-1226796	Ce2ZnSb4	Ca	1.21
26	mp-631551	MnAlTc	Ca	1.23
27	mp-133	Sb	Ca	1.24
28	mp-1190582	Mg6NbH16	Ca	1.25
29	mp-1191096	Mg6VH16	Ca	1.26
30	mp-1096950	Fe	Ca	1.27
31	mp-1014230	TiZn	Ca	1.32
32	mp-1179605	Sb	Ca	1.37
33	mp-1191566	Zn6Sb5	Ca	1.38
34	mp-1228713	Al4Ni15	Ca	1.41
35	mvc-14876	Ba2Ti3O8	Ca	1.42
36	mp-1191852	Mg6TiH16	Ca	1.45
37	mp-1094565	MgSb	Ca	1.47
38	mp-589	TbFe2	Ca	1.50
39	mp-12627	Nb3S4	Ca	1.50
40	mp-7564	Nb3Te4	Ca	1.50
41	mp-1048199	BaTi4O7	Ca	1.51
42	mp-1039305	MgBi	Ca	1.53
43	mp-21050	UFe2	Ca	1.54
44	mp-7162	Sn	Ca	1.55
45	mp-1048501	Ba2W3O7	Ca	1.56
46	mvc-14816	Al(CuS2)3	Ca	1.58
47	mp-21594	Ca9Zn4Sb9	Ca	1.65
48	mvc-11780	MoS2	Ca	1.65
49	mp-929	ZrCo2	Ca	1.68
50	mvc-12404	TiO2	Ca	1.70
51	mp-1056004	Mo	Ca	1.71
52	mp-8637	Mo	Ca	1.72
53	mp-11503	MnZn	Ca	1.73
54	mp-1009813	SiSn	Ca	1.73
55	mp-129	Mo	Ca	1.74
56	mp-21021	Mo3Se4	Ca	1.76
57	mp-561	Nb3Se4	Ca	1.76
58	mp-1383	UCo2	Ca	1.77
59	mp-2250	ZrNi2	Ca	1.79
60	mp-1008728	Ni	Ca	1.84
61	mvc-1332	BaV4O7	Ca	1.85
62	mp-754767	Fe3(SnS4)2	Ca	1.86
63	mp-1221647	MnCr	Ca	1.87
64	mp-1046350	Ba2TlW2O7	Ca	1.89
65	mp-1048112	Ba2V3O8	Ca	1.92
66	mp-1045898	V9O13	Ca	1.93

67	mp-1094669	MgSn	Ca	1.93
68	mp-1009730	Ca2Sn	Ca	1.93
69	mvc-1364	Ba2V3O7	Ca	1.95
70	mp-1147769	Cu2GeS4	Ca	1.95
71	mvc-157	Mg(WO2)4	Ca	1.95
72	mp-1045011	Sr2YCr2O7	Ca	1.98
73	mp-637219	Mo4O5	Ca	2.02
74	mvc-12090	Al5(BiS4)3	Ca	2.03
75	mp-1044267	TiV(PO4)3	Ca	2.04
76	mp-23	Ni	Ca	2.09
77	mp-542633	GdCo2	Ca	2.10
78	mvc-4354	SiWO4	Ca	2.11
79	mp-1143521	Si2WO6	Ca	2.13
80	mvc-13600	AlBiSe4	Ca	2.18
81	mp-1048194	Ba2W3O8	Ca	2.19
82	mp-1112	CeCo2	Ca	2.22
83	mvc-12231	MgV4O8	Ca	2.23
84	mp-1094572	Mg2Sb	Ca	2.27
85	mvc-12745	Rb6Al4(Sb2O7)3	Ca	2.28
86	mp-1047245	Sr2YFe2O7	Ca	2.30
87	mp-1046025	Mg(MoO2)4	Ca	2.32
88	mp-16722	Al10V	Ca	2.34
89	mvc-11306	Al13(CuS8)3	Ca	2.40
90	mvc-15048	MnNb2ZnO8	Ca	2.41
91	mvc-12595	Mn2ZnO4	Ca	2.43
92	mvc-12771	MgV2O6	Ca	2.44
93	mp-21855	VCu3Se4	Ca	2.44
94	mp-1022721	AlCu	Ca	2.44
95	mp-19529	W18O49	Ca	2.46
96	mp-1045734	MgV2O6	Ca	2.47
97	mvc-12227	Mn3Nb2O9	Ca	2.48
98	mp-1044382	TiCr(PO4)3	Ca	2.48
99	mp-1046342	Ba2TlFe2O7	Ca	2.50
100	mvc-11295	Al13(CuSe8)3	Ca	2.50
101	mp-1143876	VSiO4	Ca	2.51
102	mp-1048391	BaFe4O7	Ca	2.52
103	mvc-15230	MgV2O6	Ca	2.52
104	mp-1206438	Rb2CuF6	Ca	2.53
105	mvc-5659	SnO2	Ca	2.54
106	mvc-13329	Sr9Zn2(CuO7)2	Ca	2.56
107	mp-1343	NdNi2	Ca	2.56
108	mp-1048371	BaCr4O7	Ca	2.57
109	mp-1042978	W3O8	Ca	2.58
110	mp-547271	ReO3	Ca	2.60
111	mvc-11839	Al(CuSe2)3	Ca	2.61
112	mvc-15363	SnO2	Ca	2.61

113	mp-1041213	P4W3O14	Ca	2.62
114	mp-1046053	Ba2TlSn2O7	Ca	2.63
115	mp-1041474	Sr2YMn2O7	Ca	2.64
116	mvc-9896	SnO2	Ca	2.65
117	mvc-12134	Mn2Nb2O9	Ca	2.67
118	mp-1048539	Ba2Cr3O7	Ca	2.67
119	mvc-5236	SnO2	Ca	2.70
120	mp-1048765	Mg(SbO3)2	Ca	2.72
121	mvc-637	Re(WO4)2	Ca	2.72
122	mvc-13175	Ta2MnZnO8	Ca	2.72
123	mp-1216303	VPO5	Ca	2.72
124	mp-1003641	MgMn2O4	Ca	2.74
125	mp-1039074	MgBi	Ca	2.75
126	mvc-5310	VO2	Ca	2.75
127	mp-1041486	Ti(WO4)2	Ca	2.76
128	mp-1046192	Sn5(TeO6)3	Ca	2.77
129	mvc-11309	Cr2S5	Ca	2.77
130	mvc-14991	SrCuSO	Ca	2.78
131	mp-715479	Mo3O8	Ca	2.81
132	mp-1094498	Mg5Ti	Ca	2.81
133	mp-510748	V2O5	Ca	2.82
134	mp-1047167	Sr2YCo2O7	Ca	2.82
135	mp-1142770	SiSnO4	Ca	2.82
136	mp-1048508	BaMn4O7	Ca	2.85
137	mvc-13133	Cu2SnSe4	Ca	2.85
138	mp-1043403	Si4SnO10	Ca	2.86
139	mp-1018795	Mg2Sn	Ca	2.86
140	mvc-13180	CrSe2	Ca	2.87
141	mvc-5592	P2WO7	Ca	2.88
142	mp-656880	Y2Mn2S2O5	Ca	2.89
143	mp-1045304	Zn(SbO3)2	Ca	2.89
144	mp-89	Cr	Ca	2.89
145	mp-1042189	Ba2Sb3O8	Ca	2.90
146	mp-102	Co	Ca	2.95
147	mp-1041824	V(WO4)2	Ca	2.95
148	mp-1048188	Ba2Sn3O7	Ca	2.96
149	mvc-14274	ZnCr4O8	Ca	2.96
150	mvc-13140	Cu2GeSe4	Ca	2.97
151	mp-1045698	V2ZnO6	Ca	3.00
152	mvc-13124	Mg3V2(BiO6)2	Ca	3.00
153	mp-540258	Ti(PO3)4	Ca	3.00
154	mvc-12581	MgCr4O8	Ca	3.02
155	mp-1045634	Zn(FeO2)4	Ca	3.05
156	mvc-12789	ScMo3O8	Ca	3.06
157	mvc-14940	Ti(BiO3)2	Ca	3.06
158	mp-1041809	Ta(WO4)2	Ca	3.06

159	mp-90	Cr	Ca	3.06
160	mp-1046527	Cr5(TeO6)3	Ca	3.06
161	mvc-12603	Mg(FeO2)2	Ca	3.07
162	mp-1046936	Sr2GaCo2O7	Ca	3.10
163	mp-1042388	BiSbO5	Ca	3.13
164	mp-1143241	CrSiO4	Ca	3.14
165	mvc-5444	MnO2	Ca	3.14
166	mvc-14949	Ti(BiO3)2	Ca	3.15
167	mp-1046050	Cr5O7	Ca	3.15
168	mp-1041550	Sr2YNi2O7	Ca	3.15
169	mp-1047717	V(WO4)2	Ca	3.16
170	mp-775220	V(GeO3)2	Ca	3.16
171	mp-656884	Ni9O10	Ca	3.17
172	mvc-14071	Al5(CuO4)3	Ca	3.20
173	mp-1225007	Fe5O8	Ca	3.21
174	mp-1048511	Ba2Mn3O7	Ca	3.22
175	mp-1041693	Cr(WO4)2	Ca	3.23
176	mvc-12133	V2Zn3(P2O9)2	Ca	3.24
177	mp-1041563	Mn(WO4)2	Ca	3.24
178	mp-1041860	Te(WO4)2	Ca	3.26
179	mvc-15040	Mn13Si2(SbO14)2	Ca	3.26
180	mp-1048779	Mg(BiO3)2	Ca	3.26
181	mp-1041585	Re(WO4)2	Ca	3.27
182	mvc-11008	Ba2Fe3O8	Ca	3.27
183	mvc-11996	Zn3Bi2(PO6)2	Ca	3.28
184	mp-1042656	W3O8	Ca	3.28
185	mp-33009	MnO2	Ca	3.29
186	mp-1041577	Sn(WO4)2	Ca	3.32
187	mvc-11845	Al5(CuO4)3	Ca	3.32
188	mvc-14856	Al2(CuO2)3	Ca	3.33
189	mvc-9418	Fe13Si2(SbO14)2	Ca	3.33
190	mp-1041534	Mo(WO4)2	Ca	3.34
191	mp-1046509	Mn5(TeO6)3	Ca	3.34
192	mvc-12806	Mg3Bi2(PO6)2	Ca	3.34
193	mvc-12177	MnSiO4	Ca	3.35
194	mp-1041231	Sn3P3O13	Ca	3.35
195	mp-1047752	Sb(WO4)2	Ca	3.36
196	mvc-5268	SbAsO5	Ca	3.37
197	mp-30	Cu	Ca	3.39
198	mp-1046704	VPO5	Ca	3.40
199	mvc-12565	Mg(CoO2)4	Ca	3.41
200	mp-1041598	Fe(WO4)2	Ca	3.44
201	mvc-12570	Mg(NiO2)4	Ca	3.45
202	mp-1143147	FeSiO4	Ca	3.45
203	mp-1048179	BaCu4O7	Ca	3.45
204	mp-767563	P4WO12	Ca	3.46

205	mvc-12916	V6Zn(FeO6)4	Ca	3.46
206	mvc-13206	Al5Cu3Si6(O7F2)3	Ca	3.46
207	mvc-5626	MoAsO5	Ca	3.49
208	mvc-12282	MgV2(SiO4)3	Ca	3.50
209	mp-1045326	Zn(BiO3)2	Ca	3.50
210	mvc-11632	VBiO5	Ca	3.51
211	mvc-11924	Mg3Bi2(AsO6)2	Ca	3.52
212	mvc-14468	MgV6(FeO6)4	Ca	3.53
213	mvc-13721	Ba2Ni3O8	Ca	3.54
214	mp-1047617	Co(WO4)2	Ca	3.55
215	mp-777836	Li14Co13O28	Ca	3.55
216	mp-1048124	Ba2Cr3O8	Ca	3.57
217	mp-1094189	Mg5Sn	Ca	3.58
218	mvc-11375	Mg2Mn2(SiO4)3	Ca	3.60
219	mp-1043373	Bi2O5	Ca	3.61
220	mvc-14589	CrO2	Ca	3.62
221	mp-1048554	Ba2Ni3O7	Ca	3.62
222	mvc-13345	Al5(NiO4)3	Ca	3.64
223	mp-1221188	NaCa3Fe(SiO3)8	Ca	3.65
224	mvc-15145	Zn3Cu10(TeO6)6	Ca	3.65
225	mp-1045581	Zn(CoO2)4	Ca	3.66
226	mp-769642	Fe(CO3)2	Ca	3.67
227	mp-1041572	Bi(WO4)2	Ca	3.69
228	mp-773884	Bi19O30	Ca	3.69
229	mvc-11096	MoO3	Ca	3.70
230	mvc-11646	BaCo4O7	Ca	3.71
231	mvc-11548	CrO3	Ca	3.72
232	mp-1042304	Ni(WO4)2	Ca	3.73
233	mvc-13581	Al2Fe3(PO5)3	Ca	3.73
234	mvc-13145	Zn3Cu2(AsO4)4	Ca	3.80
235	mp-1044987	Zn(NiO2)4	Ca	3.80
236	mvc-14109	Al4(CoO4)3	Ca	3.80
237	mp-1221093	NaCaFe(SiO3)4	Ca	3.83
238	mvc-12893	Al4(NiO4)3	Ca	3.83
239	mvc-15019	V2(PO4)3	Ca	3.83
240	mp-769727	Li3(NiO2)4	Ca	3.84
241	mvc-11581	CrO2	Ca	3.85
242	mp-1039182	Mg2Bi	Ca	3.86
243	mvc-14116	Al4(CoO4)3	Ca	3.86
244	mvc-5644	VAsO5	Ca	3.87
245	mp-1044873	Bi2P2O9	Ca	3.88
246	mp-1172361	CoSiO4	Ca	3.91
247	mvc-11181	Al(CuO2)3	Ca	3.93
248	mvc-15002	Al4(FeO4)3	Ca	3.93
249	mvc-11925	MgBiPO6	Ca	3.93
250	mvc-14924	Al4(FeO4)3	Ca	3.95

251	mvc-2990	Ba2TlNi2O7	Ca	3.95
252	mvc-14138	Al2(FeO3)3	Ca	3.97
253	mvc-12287	Mg2Fe2(SiO4)3	Ca	4.02
254	mvc-11457	WO3	Ca	4.02
255	mvc-4519	SiNiO4	Ca	4.04
256	mp-644514	MnO2	Ca	4.09
257	mvc-13999	CrO3	Ca	4.09
258	mp-1197460	Al4Fe(SiO6)2	Ca	4.10
259	mp-1048172	Ba2Mn3O8	Ca	4.15
260	mp-1228752	Al4Cu15	Ca	4.19
261	mvc-13141	Al4(FeO4)3	Ca	4.22
262	mvc-12194	Al10(Bi2O9)3	Ca	4.23
263	mvc-11097	CrO3	Ca	4.29
264	mp-1048029	Ni3P3O13	Ca	4.36
265	mp-1047608	Co3(AsO4)4	Ca	4.45
266	mvc-12815	Bi6P2O15	Ca	4.47
267	mp-1221594	MnO4	Ca	4.48
268	mp-765763	Cr(SO4)2	Ca	4.50
269	mp-773979	Cr(SO4)2	Ca	4.50
270	mp-1048486	BaNi4O7	Ca	4.83
271	mvc-6713	Ni3(AsO4)4	Ca	4.94
272	mvc-14312	VF5	Ca	4.98
273	mvc-15137	Ba2ZnFe2F14	Ca	5.06
274	mvc-13128	AlFe3F15	Ca	5.06
275	mvc-13155	Mn3AlF15	Ca	5.49
276	mvc-11777	Al(BiO3)3	Ca	5.80
277	mp-1041349	BaBiF7	Ca	5.90
278	mvc-14843	Al(BiO3)3	Ca	5.90

Supplementary Table 5. Predicted electrode voltages for Mg-ion batteries.

The crystals have been used as electrodes for Ca-, Zn-, and Al-ion batteries, and we here predict their electrode voltage for Mg-ion batteries.

	entry_id	formula	working_ion	pred_voltage
1	mp-1061123	TiAl	Mg	-1.57
2	mvc-4059	TiSiO4	Mg	-0.65
3	mp-1228713	Al4Ni15	Mg	-0.41
4	mp-568345	Fe	Mg	-0.37
5	mp-2649	Zr5Sb3	Mg	-0.36
6	mp-510522	Zr5Sn3	Mg	-0.32
7	mp-1094034	Ti3C2	Mg	-0.15
8	mp-1065340	W	Mg	-0.07
9	mp-1008753	Ti2Al	Mg	-0.03
10	mp-589	TbFe2	Mg	0.00
11	mvc-11235	BiN	Mg	0.02
12	mp-1718	ZrFe2	Mg	0.05

13	mp-631551	MnAlTc	Mg	0.06
14	mp-1055908	Mn	Mg	0.06
15	mp-542633	GdCo2	Mg	0.08
16	mp-1014230	TiZn	Mg	0.09
17	mp-1008728	Ni	Mg	0.14
18	mp-7564	Nb3Te4	Mg	0.15
19	mp-971669	FeSb3	Mg	0.17
20	mp-91	W	Mg	0.21
21	mp-1112	CeCo2	Mg	0.22
22	mp-21050	UFe2	Mg	0.23
23	mp-11503	MnZn	Mg	0.25
24	mp-8637	Mo	Mg	0.26
25	mp-1383	UCo2	Mg	0.29
26	mp-1221647	MnCr	Mg	0.29
27	mp-929	ZrCo2	Mg	0.32
28	mp-129	Mo	Mg	0.40
29	mp-1226796	Ce2ZnSb4	Mg	0.41
30	mp-568806	C	Mg	0.44
31	mp-16722	Al10V	Mg	0.45
32	mp-1191566	Zn6Sb5	Mg	0.47
33	mp-10631	Sb	Mg	0.50
34	mp-21594	Ca9Zn4Sb9	Mg	0.56
35	mp-561	Nb3Se4	Mg	0.57
36	mp-1048501	Ba2W3O7	Mg	0.59
37	mvc-10945	Ca2VN3	Mg	0.59
38	mvc-11274	CaCoN2	Mg	0.59
39	mvc-14421	BaCa(CoN2)2	Mg	0.60
40	mvc-11744	Ca(TiS2)4	Mg	0.62
41	mvc-14816	Al(CuS2)3	Mg	0.64
42	mp-2250	ZrNi2	Mg	0.64
43	mp-1009730	Ca2Sn	Mg	0.67
44	mvc-2846	W5O7	Mg	0.71
45	mvc-11104	Ca2CrN3	Mg	0.73
46	mp-1045759	Ti5O7	Mg	0.78
47	mp-12627	Nb3S4	Mg	0.79
48	mvc-11162	NiN	Mg	0.80
49	mvc-11164	Ca11(FeN5)2	Mg	0.85
50	mp-1147769	Cu2GeS4	Mg	0.85
51	mp-1048199	BaTi4O7	Mg	0.88
52	mp-1046350	Ba2TlW2O7	Mg	0.89
53	mvc-13041	Ca11(MnN5)2	Mg	0.90
54	mvc-14842	BaCa3(CuN2)2	Mg	0.90
55	mvc-12176	CaTi4O8	Mg	0.92
56	mvc-4354	SiWO4	Mg	0.97
57	mvc-13841	CuN	Mg	0.97
58	mp-2156	TiS2	Mg	0.99

59	mvc-14876	Ba2Ti3O8	Mg	1.00
60	mvc-2118	WO2	Mg	1.02
61	mvc-14086	Ca5(MnN3)2	Mg	1.05
62	mp-1048593	Ca(TiS2)2	Mg	1.06
63	mvc-12090	Al5(BiS4)3	Mg	1.07
64	mp-1046039	V5O7	Mg	1.07
65	mvc-13600	AlBiSe4	Mg	1.08
66	mp-90	Cr	Mg	1.08
67	mvc-1364	Ba2V3O7	Mg	1.10
68	mvc-11780	MoS2	Mg	1.14
69	mp-754767	Fe3(SnS4)2	Mg	1.18
70	mp-1045011	Sr2YCr2O7	Mg	1.18
71	mvc-93	Ca(MnS2)4	Mg	1.22
72	mvc-13329	Sr9Zn2(CuO7)2	Mg	1.25
73	mp-1143876	VSiO4	Mg	1.29
74	mvc-1332	BaV4O7	Mg	1.29
75	mvc-15882	Mo2O5	Mg	1.29
76	mp-637219	Mo4O5	Mg	1.30
77	mvc-15011	Ca3Nd4Nb6(FeO14)2	Mg	1.31
78	mp-608555	Cs2SnCl6	Mg	1.32
79	mp-1022721	AlCu	Mg	1.32
80	mvc-11839	Al(CuSe2)3	Mg	1.33
81	mvc-11295	Al13(CuSe8)3	Mg	1.35
82	mp-1143521	Si2WO6	Mg	1.36
83	mp-1214031	CaC4	Mg	1.40
84	mp-30	Cu	Mg	1.41
85	mvc-12404	TiO2	Mg	1.41
86	mvc-13572	Mn2Be3(SiO4)3	Mg	1.42
87	mp-19529	W18O49	Mg	1.43
88	mp-1048194	Ba2W3O8	Mg	1.44
89	mp-1047245	Sr2YFe2O7	Mg	1.45
90	mvc-15895	W2O5	Mg	1.47
91	mp-1048371	BaCr4O7	Mg	1.47
92	mvc-12918	Sb5S3O5	Mg	1.53
93	mp-19443	WO3	Mg	1.54
94	mvc-12321	CaSb2S5	Mg	1.55
95	mp-1048112	Ba2V3O8	Mg	1.56
96	mvc-13133	Cu2SnSe4	Mg	1.57
97	mvc-11306	Al13(CuS8)3	Mg	1.57
98	mvc-12745	Rb6Al4(Sb2O7)3	Mg	1.61
99	mvc-5346	TiP2O7	Mg	1.61
100	mvc-14991	SrCuSO	Mg	1.64
101	mp-1206438	Rb2CuF6	Mg	1.67
102	mp-1046342	Ba2TlFe2O7	Mg	1.67
103	mvc-13140	Cu2GeSe4	Mg	1.70
104	mvc-15048	MnNb2ZnO8	Mg	1.70

105	mvc-12595	Mn2ZnO4	Mg	1.74
106	mp-1116820	MoWO6	Mg	1.75
107	mvc-12227	Mn3Nb2O9	Mg	1.75
108	mvc-12286	Ca2Nb2CoO9	Mg	1.76
109	mp-1216303	VPO5	Mg	1.76
110	mp-1041474	Sr2YMn2O7	Mg	1.77
111	mp-1227103	CaNb4O14	Mg	1.84
112	mvc-12077	VO2	Mg	1.85
113	mp-1048391	BaFe4O7	Mg	1.87
114	mvc-13677	MoO2	Mg	1.89
115	mp-1047300	SbO2	Mg	1.93
116	mp-1142770	SiSnO4	Mg	1.93
117	mp-1143241	CrSiO4	Mg	1.93
118	mp-1045293	Ca(SbO3)2	Mg	1.93
119	mvc-10909	Ca3Ta2Mn2O12	Mg	1.95
120	mp-1046053	Ba2TlSn2O7	Mg	1.97
121	mvc-11183	SrCuBiO4	Mg	1.99
122	mvc-12134	Mn2Nb2O9	Mg	2.00
123	mp-1046617	Sr2MnSO3	Mg	2.00
124	mp-1048539	Ba2Cr3O7	Mg	2.00
125	mvc-11373	CaMnWO6	Mg	2.01
126	mp-1044716	SbO2	Mg	2.01
127	mp-1047167	Sr2YCo2O7	Mg	2.02
128	mvc-5659	SnO2	Mg	2.04
129	mp-1046050	Cr5O7	Mg	2.04
130	mvc-11942	CaTi2Fe2(PO4)6	Mg	2.05
131	mp-1045634	Zn(FeO2)4	Mg	2.06
132	mvc-5592	P2WO7	Mg	2.06
133	mvc-11086	V2O5	Mg	2.09
134	mvc-15363	SnO2	Mg	2.10
135	mvc-7566	Ta2CoO7	Mg	2.10
136	mvc-12039	Fe5O7	Mg	2.11
137	mvc-13175	Ta2MnZnO8	Mg	2.12
138	mp-1046936	Sr2GaCo2O7	Mg	2.13
139	mvc-11947	CaV2O6	Mg	2.13
140	mp-1044910	VPO4	Mg	2.14
141	mvc-11828	Ca2CuIrO6	Mg	2.14
142	mvc-14243	CaCoO3	Mg	2.14
143	mp-1046066	Mn5O7	Mg	2.14
144	mvc-15237	Ba4CaCu6(HgO8)2	Mg	2.15
145	mvc-637	Re(WO4)2	Mg	2.15
146	mp-1045698	V2ZnO6	Mg	2.15
147	mvc-14071	Al5(CuO4)3	Mg	2.16
148	mvc-11950	CaNd2Ti2Mn2O12	Mg	2.18
149	mvc-14274	ZnCr4O8	Mg	2.20
150	mvc-11845	Al5(CuO4)3	Mg	2.21

151	mp-776137	VO2	Mg	2.23
152	mvc-13032	Ba2Cu2HgO6	Mg	2.23
153	mp-1045304	Zn(SbO3)2	Mg	2.24
154	mvc-11852	Ba2CaTl2(CuO3)4	Mg	2.24
155	mp-1041486	Ti(WO4)2	Mg	2.25
156	mvc-13206	Al5Cu3Si6(O7F2)3	Mg	2.29
157	mvc-10923	Ca(FeO2)2	Mg	2.29
158	mvc-13117	CaLa2Ti2Cr2O12	Mg	2.29
159	mp-1042407	CuW2O7	Mg	2.30
160	mp-1228752	Al4Cu15	Mg	2.31
161	mvc-12789	ScMo3O8	Mg	2.32
162	mvc-11781	CaTi2F10	Mg	2.32
163	mvc-12889	Ca3Co2(TeO6)2	Mg	2.33
164	mvc-14856	Al2(CuO2)3	Mg	2.33
165	mp-715479	Mo3O8	Mg	2.33
166	mp-1041824	V(WO4)2	Mg	2.33
167	mp-1042189	Ba2Sb3O8	Mg	2.33
168	mvc-12760	CaNiWO6	Mg	2.33
169	mvc-13028	CaCu2F8	Mg	2.34
170	mvc-12038	Mn4(SiO3)5	Mg	2.35
171	mp-1048188	Ba2Sn3O7	Mg	2.37
172	mvc-14237	CaCoWO6	Mg	2.37
173	mvc-14832	Ca2CuRhO6	Mg	2.38
174	mp-1041550	Sr2YNi2O7	Mg	2.38
175	mvc-14929	CaLa2Ti2Mn2O12	Mg	2.39
176	mvc-10908	Ca3Mn2(SbO6)2	Mg	2.39
177	mvc-12304	V2P2O9	Mg	2.41
178	mp-1043235	V(GeO3)2	Mg	2.43
179	mvc-11885	Ba4CaTl4(Cu3O10)2	Mg	2.43
180	mvc-10916	CaFeWO6	Mg	2.43
181	mvc-11334	Ca3(CuO3)2	Mg	2.43
182	mvc-14106	CaVBiO6	Mg	2.44
183	mvc-13047	Ba2CaTl2(CuO3)4	Mg	2.46
184	mvc-11996	Zn3Bi2(PO6)2	Mg	2.46
185	mvc-12133	V2Zn3(P2O9)2	Mg	2.48
186	mvc-12020	CaMnSi2O7	Mg	2.49
187	mvc-13123	CaFeReO6	Mg	2.49
188	mvc-11008	Ba2Fe3O8	Mg	2.50
189	mp-1046082	Co5O7	Mg	2.51
190	mvc-10959	VBiO5	Mg	2.51
191	mvc-9418	Fe13Si2(SbO14)2	Mg	2.51
192	mp-1041809	Ta(WO4)2	Mg	2.53
193	mp-1147673	Cu3O4	Mg	2.53
194	mvc-12278	CaV4(CuO7)2	Mg	2.53
195	mp-1043389	NiP2WO9	Mg	2.53
196	mvc-12177	MnSiO4	Mg	2.53

197	mp-1048508	BaMn4O7	Mg	2.55
198	mp-543057	MnO2	Mg	2.55
199	mvc-13721	Ba2Ni3O8	Mg	2.55
200	mvc-14981	Ca3Fe2(SbO6)2	Mg	2.56
201	mvc-11834	BaTlCuO4	Mg	2.56
202	mp-656884	Ni9O10	Mg	2.56
203	mvc-14940	Ti(BiO3)2	Mg	2.57
204	mvc-15040	Mn13Si2(SbO14)2	Mg	2.57
205	mvc-11930	Ca3Mn2(GaO5)2	Mg	2.58
206	mvc-14984	Ca3Co2(RhO6)2	Mg	2.58
207	mp-1041563	Mn(WO4)2	Mg	2.58
208	mp-1047717	V(WO4)2	Mg	2.59
209	mvc-14254	Ca3Fe2(RhO6)2	Mg	2.60
210	mvc-14949	Ti(BiO3)2	Mg	2.60
211	mp-1044028	LaFeBiO6	Mg	2.60
212	mvc-10912	CaMnIrO6	Mg	2.60
213	mvc-11007	CaFeMoO6	Mg	2.61
214	mvc-14986	CaNiWO6	Mg	2.61
215	mp-1143147	FeSiO4	Mg	2.62
216	mp-1048179	BaCu4O7	Mg	2.63
217	mp-19395	MnO2	Mg	2.65
218	mvc-12611	CaCr4O8	Mg	2.65
219	mvc-14096	Cu3(GeO3)4	Mg	2.66
220	mvc-12916	V6Zn(FeO6)4	Mg	2.66
221	mvc-12302	Ca8Cr(PO4)7	Mg	2.66
222	mvc-12280	Ba2CaV2(P2O9)2	Mg	2.66
223	mp-1225007	Fe5O8	Mg	2.67
224	mp-1048511	Ba2Mn3O7	Mg	2.68
225	mp-1042656	W3O8	Mg	2.69
226	mp-1041693	Cr(WO4)2	Mg	2.70
227	mp-1043195	V(GeO3)2	Mg	2.70
228	mvc-10961	V4O9	Mg	2.72
229	mp-782692	Mn7O12	Mg	2.72
230	mvc-15035	Ca3Ga2(FeO5)2	Mg	2.74
231	mvc-12787	CaCu2(Si2O5)4	Mg	2.74
232	mp-1041585	Re(WO4)2	Mg	2.74
233	mvc-13694	La2MoO6	Mg	2.76
234	mvc-14970	Ti4(FeO4)3	Mg	2.78
235	mp-851050	Ca9Co(PO4)7	Mg	2.78
236	mvc-13642	VF4	Mg	2.80
237	mp-1048554	Ba2Ni3O7	Mg	2.80
238	mvc-15207	Ta2Bi2O9	Mg	2.81
239	mp-1041534	Mo(WO4)2	Mg	2.81
240	mvc-5774	CrWO6	Mg	2.84
241	mvc-15204	Ta2Bi2O9	Mg	2.88
242	mvc-10906	Ca2MnNiO6	Mg	2.90

243	mvc-12807	CaMnFeO5	Mg	2.90
244	mp-1041577	Sn(WO4)2	Mg	2.90
245	mp-1117500	SnF4	Mg	2.90
246	mp-1041860	Te(WO4)2	Mg	2.92
247	mp-1041598	Fe(WO4)2	Mg	2.92
248	mp-1045581	Zn(CoO2)4	Mg	2.92
249	mp-1047752	Sb(WO4)2	Mg	2.93
250	mvc-13126	Ca5Sc2(CoO6)2	Mg	2.94
251	mp-1048124	Ba2Cr3O8	Mg	2.94
252	mvc-13345	Al5(NiO4)3	Mg	2.95
253	mp-1041470	CrCuO4	Mg	2.95
254	mvc-13172	Ba4CaV4Cu2F28	Mg	2.96
255	mp-765928	VF5	Mg	2.97
256	mvc-14980	CaMn2O5	Mg	2.97
257	mp-1045326	Zn(BiO3)2	Mg	2.97
258	mvc-15145	Zn3Cu10(TeO6)6	Mg	2.98
259	mp-1046591	Ba2Tl2Ni3O10	Mg	2.98
260	mp-1041231	Sn3P3O13	Mg	2.99
261	mp-540363	VP2O7	Mg	2.99
262	mp-1045327	Ca(BiO3)2	Mg	2.99
263	mvc-11380	V2CoO7	Mg	3.00
264	mvc-14253	Ca3Mn2O7	Mg	3.01
265	mp-1048924	FePO4	Mg	3.02
266	mvc-11096	MoO3	Mg	3.04
267	mvc-11181	Al(CuO2)3	Mg	3.06
268	mp-1047386	BiO2	Mg	3.06
269	mvc-8434	Cr(GeO3)2	Mg	3.07
270	mvc-13581	Al2Fe3(PO5)3	Mg	3.07
271	mvc-12258	Ca2Mn2(SiO4)3	Mg	3.09
272	mp-1047617	Co(WO4)2	Mg	3.09
273	mvc-14109	Al4(CoO4)3	Mg	3.10
274	mvc-11865	CaCoSi2O7	Mg	3.10
275	mvc-6353	MnO2	Mg	3.10
276	mp-1221467	MoO4	Mg	3.11
277	mp-1044987	Zn(NiO2)4	Mg	3.12
278	mvc-11916	Ca2La5Mn7NiO24	Mg	3.15
279	mvc-14116	Al4(CoO4)3	Mg	3.19
280	mvc-11883	Ca3Cu6(PO4)8	Mg	3.20
281	mvc-2990	Ba2TlNi2O7	Mg	3.21
282	mvc-12893	Al4(NiO4)3	Mg	3.22
283	mvc-13145	Zn3Cu2(AsO4)4	Mg	3.22
284	mvc-15002	Al4(FeO4)3	Mg	3.23
285	mp-1043651	BiSbO5	Mg	3.24
286	mvc-12905	FeO2	Mg	3.25
287	mp-1043556	SbPO5	Mg	3.25
288	mp-1172361	CoSiO4	Mg	3.25

289	mvc-11548	CrO3	Mg	3.26
290	mp-1044170	CrPO5	Mg	3.26
291	mvc-11457	WO3	Mg	3.26
292	mvc-12050	NiO2	Mg	3.26
293	mvc-14924	Al4(FeO4)3	Mg	3.26
294	mp-1042304	Ni(WO4)2	Mg	3.28
295	mp-1042873	Sn(GeO3)2	Mg	3.29
296	mp-1197460	Al4Fe(SiO6)2	Mg	3.29
297	mvc-8359	Cr(GeO3)2	Mg	3.30
298	mp-1116784	CoO2	Mg	3.30
299	mp-1041572	Bi(WO4)2	Mg	3.30
300	mvc-11646	BaCo4O7	Mg	3.31
301	mvc-13999	CrO3	Mg	3.32
302	mp-1221542	MnO2	Mg	3.33
303	mp-1117519	Cr2O5	Mg	3.33
304	mvc-4519	SiNiO4	Mg	3.34
305	mp-1047904	Cr3P3O13	Mg	3.34
306	mp-773884	Bi19O30	Mg	3.34
307	mp-775128	Fe3Sb(PO4)6	Mg	3.34
308	mp-1040999	CuTeO4	Mg	3.36
309	mvc-15457	La2CrO6	Mg	3.38
310	mvc-14138	Al2(FeO3)3	Mg	3.40
311	mp-771678	NaFe2(SiO3)4	Mg	3.40
312	mvc-14848	CaCu2(P2O7)2	Mg	3.40
313	mp-766786	VF5	Mg	3.43
314	mp-1048172	Ba2Mn3O8	Mg	3.44
315	mvc-10979	CaCu2(GeO3)4	Mg	3.45
316	mvc-12739	CaCu2(GeO3)4	Mg	3.45
317	mvc-13490	Bi2O5	Mg	3.47
318	mp-1043461	NiSbP2O9	Mg	3.47
319	mp-1044873	Bi2P2O9	Mg	3.48
320	mvc-12194	Al10(Bi2O9)3	Mg	3.52
321	mp-1047829	Ba(NiO2)4	Mg	3.53
322	mvc-13059	Ca3Cu6(AsO4)8	Mg	3.54
323	mp-673105	Cu3(P2O7)2	Mg	3.54
324	mvc-10933	CaLa2Mn2(FeO6)2	Mg	3.59
325	mvc-12271	Ca2Fe2(SiO4)3	Mg	3.59
326	mp-540267	CrP2O7	Mg	3.60
327	mvc-11848	CaBiAsO6	Mg	3.60
328	mp-694636	MnP2O7	Mg	3.61
329	mp-1041988	CoO2	Mg	3.62
330	mvc-13141	Al4(FeO4)3	Mg	3.64
331	mp-1042286	Co(SiO3)2	Mg	3.66
332	mp-1041261	Bi3P3O13	Mg	3.66
333	mp-1044399	Mn(GeO3)2	Mg	3.67
334	mp-1042331	Mn(SiO3)2	Mg	3.67

335	mvc-11097	CrO3	Mg	3.68
336	mp-540321	FeP2O7	Mg	3.69
337	mvc-11862	CaCu2(As2O7)2	Mg	3.70
338	mp-1044639	Fe(GeO3)2	Mg	3.72
339	mvc-7342	Si2NiO6	Mg	3.74
340	mp-1043501	Fe(GeO3)2	Mg	3.75
341	mvc-2979	MnF4	Mg	3.76
342	mp-1041341	BaSbF7	Mg	3.78
343	mvc-13941	CoF4	Mg	3.80
344	mvc-10920	CaFe2F10	Mg	3.82
345	mp-1043383	Mn(GeO3)2	Mg	3.83
346	mp-1041443	Cr4O9	Mg	3.85
347	mvc-10914	CrP2O7	Mg	3.88
348	mp-1042757	CrAs2O7	Mg	3.96
349	mvc-8361	Co(GeO3)2	Mg	4.01
350	mvc-13128	AlFe3F15	Mg	4.02
351	mp-1043245	Co(GeO3)2	Mg	4.03
352	mp-1043444	Ni(GeO3)2	Mg	4.08
353	mvc-14958	Ba2CaCr2F14	Mg	4.08
354	mp-1043316	Ni(GeO3)2	Mg	4.10
355	mvc-15137	Ba2ZnFe2F14	Mg	4.11
356	mp-1047608	Co3(AsO4)4	Mg	4.18
357	mvc-3813	CrF5	Mg	4.19
358	mp-540262	CoP2O7	Mg	4.25
359	mvc-12815	Bi6P2O15	Mg	4.30
360	mp-1221594	MnO4	Mg	4.32
361	mvc-12753	CaMn2F10	Mg	4.36
362	mp-1048486	BaNi4O7	Mg	4.37
363	mp-1044234	Ni2P2O9	Mg	4.38
364	mvc-13155	Mn3AlF15	Mg	4.42
365	mp-1043572	BiPO5	Mg	4.51
366	mp-540273	NiP2O7	Mg	4.55
367	mvc-15217	Bi3(PO5)2	Mg	4.68
368	mvc-11777	Al(BiO3)3	Mg	6.01
369	mvc-14843	Al(BiO3)3	Mg	6.02

Supplementary Table 6. Predicted electrode voltages for Zn-ion batteries.

The crystals have been used as electrodes for Mg-, Ca-, and Al-ion batteries, and we here predict their electrode voltage for Zn-ion batteries.

	entry_id	formula	working_ion	pred_voltage
1	mvc-4059	TiSiO4	Zn	-2.19
2	mp-1061123	TiAl	Zn	-2.07
3	mp-1094034	Ti3C2	Zn	-0.50
4	mp-8634	Mn	Zn	-0.46
5	mp-1047986	MgTi4O8	Zn	-0.43

6	mvc-11744	Ca(TiS2)4	Zn	-0.30
7	mp-8632	V	Zn	-0.30
8	mvc-12176	CaTi4O8	Zn	-0.28
9	mp-568345	Fe	Zn	-0.25
10	mp-1065340	W	Zn	-0.23
11	mvc-4354	SiWO4	Zn	-0.21
12	mvc-11235	BiN	Zn	-0.20
13	mp-568806	C	Zn	-0.20
14	mp-91	W	Zn	-0.19
15	mp-569358	Bi	Zn	-0.16
16	mvc-157	Mg(WO2)4	Zn	-0.16
17	mp-6985	Ti	Zn	-0.13
18	mvc-2846	W5O7	Zn	-0.12
19	mp-1055908	Mn	Zn	-0.12
20	mp-23152	Bi	Zn	-0.08
21	mp-1047232	WO2	Zn	-0.07
22	mp-1096950	Fe	Zn	-0.06
23	mp-1221647	MnCr	Zn	-0.01
24	mp-8636	Nb	Zn	0.03
25	mp-631551	MnAlTc	Zn	0.04
26	mvc-14816	Al(CuS2)3	Zn	0.04
27	mp-1048199	BaTi4O7	Zn	0.04
28	mp-567597	Bi	Zn	0.06
29	mp-1143876	VSiO4	Zn	0.06
30	mp-547271	ReO3	Zn	0.09
31	mp-21021	Mo3Se4	Zn	0.10
32	mp-971669	FeSb3	Zn	0.10
33	mvc-11274	CaCoN2	Zn	0.10
34	mp-1228713	Al4Ni15	Zn	0.10
35	mp-1042291	WO2	Zn	0.10
36	mp-80	Sb	Zn	0.12
37	mp-1045898	V9O13	Zn	0.12
38	mvc-15882	Mo2O5	Zn	0.13
39	mvc-10945	Ca2VN3	Zn	0.13
40	mvc-1332	BaV4O7	Zn	0.15
41	mp-1094371	MgTi2	Zn	0.15
42	mvc-14421	BaCa(CoN2)2	Zn	0.15
43	mp-129	Mo	Zn	0.15
44	mvc-13572	Mn2Be3(SiO4)3	Zn	0.16
45	mvc-14876	Ba2Ti3O8	Zn	0.17
46	mp-1048501	Ba2W3O7	Zn	0.17
47	mp-1046654	Sr2CrSO3	Zn	0.18
48	mp-1056004	Mo	Zn	0.18
49	mvc-15011	Ca3Nd4Nb6(FeO14)2	Zn	0.21
50	mp-133	Sb	Zn	0.22
51	mp-568610	Bi	Zn	0.22

52	mp-1048371	BaCr4O7	Zn	0.23
53	mp-1112	CeCo2	Zn	0.23
54	mvc-11104	Ca2CrN3	Zn	0.25
55	mp-1179605	Sb	Zn	0.25
56	mp-1039305	MgBi	Zn	0.25
57	mp-2164	Mo3S4	Zn	0.26
58	mp-1045011	Sr2YCr2O7	Zn	0.27
59	mvc-11231	SbN	Zn	0.27
60	mp-1190582	Mg6NbH16	Zn	0.27
61	mp-1097924	MgSb	Zn	0.28
62	mp-1046350	Ba2TlW2O7	Zn	0.28
63	mp-7162	Sn	Zn	0.28
64	mp-2156	TiS2	Zn	0.30
65	mvc-14842	BaCa3(CuN2)2	Zn	0.31
66	mp-7761	Sb	Zn	0.31
67	mvc-93	Ca(MnS2)4	Zn	0.33
68	mvc-11164	Ca11(FeN5)2	Zn	0.34
69	mvc-13041	Ca11(MnN5)2	Zn	0.34
70	mp-1022721	AlCu	Zn	0.35
71	mvc-15895	W2O5	Zn	0.35
72	mvc-1364	Ba2V3O7	Zn	0.36
73	mp-623511	Sn	Zn	0.36
74	mvc-12231	MgV4O8	Zn	0.41
75	mp-1191096	Mg6VH16	Zn	0.41
76	mp-1191852	Mg6TiH16	Zn	0.43
77	mp-117	Sn	Zn	0.44
78	mp-1048593	Ca(TiS2)2	Zn	0.44
79	mp-1142770	SiSnO4	Zn	0.44
80	mvc-11780	MoS2	Zn	0.46
81	mvc-12745	Rb6Al4(Sb2O7)3	Zn	0.48
82	mvc-14086	Ca5(MnN3)2	Zn	0.49
83	mvc-13600	AlBiSe4	Zn	0.50
84	mp-1094565	MgSb	Zn	0.50
85	mp-1343	NdNi2	Zn	0.51
86	mp-89	Cr	Zn	0.53
87	mvc-12771	MgV2O6	Zn	0.55
88	mvc-11839	Al(CuSe2)3	Zn	0.57
89	mp-102	Co	Zn	0.58
90	mvc-12286	Ca2Nb2CoO9	Zn	0.59
91	mp-1009813	SiSn	Zn	0.59
92	mp-1048391	BaFe4O7	Zn	0.60
93	mp-1046584	Ba2Tl2W3O10	Zn	0.61
94	mp-90	Cr	Zn	0.62
95	mp-1143241	CrSiO4	Zn	0.62
96	mp-1227103	CaNb4O14	Zn	0.64
97	mvc-12918	Sb5S3O5	Zn	0.64

98	mp-1045293	Ca(SbO3)2	Zn	0.65
99	mvc-10909	Ca3Ta2Mn2O12	Zn	0.65
100	mvc-15230	MgV2O6	Zn	0.65
101	mp-1045734	MgV2O6	Zn	0.65
102	mp-1047245	Sr2YFe2O7	Zn	0.66
103	mp-1116820	MoWO6	Zn	0.66
104	mp-1046342	Ba2TlFe2O7	Zn	0.66
105	mvc-11942	CaTi2Fe2(PO4)6	Zn	0.67
106	mp-1046939	BaTl(WO3)2	Zn	0.68
107	mp-30	Cu	Zn	0.68
108	mp-1046025	Mg(MoO2)4	Zn	0.69
109	mvc-11295	Al13(CuSe8)3	Zn	0.72
110	mp-1048765	Mg(SbO3)2	Zn	0.73
111	mvc-11950	CaNd2Ti2Mn2O12	Zn	0.75
112	mvc-11086	V2O5	Zn	0.75
113	mp-1048112	Ba2V3O8	Zn	0.76
114	mp-1041474	Sr2YMn2O7	Zn	0.76
115	mvc-14071	Al5(CuO4)3	Zn	0.77
116	mp-1048194	Ba2W3O8	Zn	0.77
117	mp-540180	Cr3(P2O7)2	Zn	0.77
118	mvc-11183	SrCuBiO4	Zn	0.78
119	mp-1041486	Ti(WO4)2	Zn	0.78
120	mvc-11373	CaMnWO6	Zn	0.79
121	mvc-11845	Al5(CuO4)3	Zn	0.80
122	mvc-12090	Al5(BiS4)3	Zn	0.80
123	mp-540258	Ti(PO3)4	Zn	0.80
124	mp-1044910	VPO4	Zn	0.80
125	mvc-12321	CaSb2S5	Zn	0.82
126	mp-16722	Al10V	Zn	0.82
127	mp-1046053	Ba2TlSn2O7	Zn	0.82
128	mvc-11828	Ca2CuIrO6	Zn	0.82
129	mvc-13206	Al5Cu3Si6(O7F2)3	Zn	0.83
130	mvc-15486	W3O8	Zn	0.83
131	mp-608555	Cs2SnCl6	Zn	0.83
132	mp-1214031	CaC4	Zn	0.84
133	mvc-13117	CaLa2Ti2Cr2O12	Zn	0.84
134	mp-1047300	SbO2	Zn	0.85
135	mvc-637	Re(WO4)2	Zn	0.86
136	mp-1094669	MgSn	Zn	0.86
137	mp-1046942	Nb2MoO8	Zn	0.87
138	mvc-15991	Mo3O8	Zn	0.87
139	mvc-14929	CaLa2Ti2Mn2O12	Zn	0.88
140	mp-1045826	Cr9O13	Zn	0.90
141	mvc-11306	Al13(CuS8)3	Zn	0.91
142	mp-1046704	VPO5	Zn	0.91
143	mp-1047167	Sr2YCo2O7	Zn	0.91

144	mp-1044716	SbO2	Zn	0.92
145	mvc-11947	CaV2O6	Zn	0.92
146	mvc-11334	Ca3(CuO3)2	Zn	0.94
147	mp-1048539	Ba2Cr3O7	Zn	0.95
148	mvc-10908	Ca3Mn2(SbO6)2	Zn	0.95
149	mvc-12302	Ca8Cr(PO4)7	Zn	0.95
150	mvc-12280	Ba2CaV2(P2O9)2	Zn	0.95
151	mvc-11852	Ba2CaTl2(CuO3)4	Zn	0.96
152	mp-1046066	Mn5O7	Zn	0.97
153	mp-1041824	V(WO4)2	Zn	0.97
154	mvc-7566	Ta2CoO7	Zn	0.97
155	mvc-13028	CaCu2F8	Zn	0.97
156	mp-1046936	Sr2GaCo2O7	Zn	0.98
157	mvc-11309	Cr2S5	Zn	0.98
158	mvc-11781	CaTi2F10	Zn	0.99
159	mp-1048179	BaCu4O7	Zn	0.99
160	mvc-14856	Al2(CuO2)3	Zn	0.99
161	mp-1047075	MoO2	Zn	1.01
162	mvc-12038	Mn4(SiO3)5	Zn	1.01
163	mvc-12889	Ca3Co2(TeO6)2	Zn	1.01
164	mvc-14243	CaCoO3	Zn	1.02
165	mp-1041292	Ba(CoO2)4	Zn	1.02
166	mvc-15237	Ba4CaCu6(HgO8)2	Zn	1.03
167	mp-1003641	MgMn2O4	Zn	1.05
168	mp-851050	Ca9Co(PO4)7	Zn	1.06
169	mp-1206438	Rb2CuF6	Zn	1.07
170	mvc-12020	CaMnSi2O7	Zn	1.08
171	mvc-13124	Mg3V2(BiO6)2	Zn	1.08
172	mp-1043235	V(GeO3)2	Zn	1.09
173	mvc-12760	CaNiWO6	Zn	1.09
174	mvc-14832	Ca2CuRhO6	Zn	1.09
175	mvc-12177	MnSiO4	Zn	1.09
176	mp-1046652	Sr2FeSO3	Zn	1.09
177	mvc-14106	CaVBiO6	Zn	1.10
178	mvc-12278	CaV4(CuO7)2	Zn	1.11
179	mp-1041809	Ta(WO4)2	Zn	1.12
180	mp-1040783	Ho(SbO3)2	Zn	1.12
181	mvc-12581	MgCr4O8	Zn	1.13
182	mvc-12806	Mg3Bi2(PO6)2	Zn	1.13
183	mvc-13047	Ba2CaTl2(CuO3)4	Zn	1.13
184	mvc-13032	Ba2Cu2HgO6	Zn	1.14
185	mvc-11633	VPO5	Zn	1.14
186	mvc-10923	Ca(FeO2)2	Zn	1.14
187	mp-1046932	BaTl(NiO3)2	Zn	1.15
188	mvc-13123	CaFeReO6	Zn	1.15
189	mvc-14237	CaCoWO6	Zn	1.15

190	mvc-11885	Ba4CaTl4(Cu3O10)2	Zn	1.16
191	mvc-14981	Ca3Fe2(SbO6)2	Zn	1.16
192	mp-1041550	Sr2YNi2O7	Zn	1.16
193	mp-1046608	Sr3Co2S2O5	Zn	1.19
194	mvc-14986	CaNiWO6	Zn	1.19
195	mp-656880	Y2Mn2S2O5	Zn	1.20
196	mp-1047717	V(WO4)2	Zn	1.20
197	mvc-12787	CaCu2(Si2O5)4	Zn	1.20
198	mp-543057	MnO2	Zn	1.20
199	mvc-14096	Cu3(GeO3)4	Zn	1.21
200	mp-1041563	Mn(WO4)2	Zn	1.21
201	mp-33009	MnO2	Zn	1.21
202	mvc-12282	MgV2(SiO4)3	Zn	1.23
203	mvc-10961	V4O9	Zn	1.23
204	mvc-10916	CaFeWO6	Zn	1.24
205	mp-1143147	FeSiO4	Zn	1.24
206	mp-1048508	BaMn4O7	Zn	1.24
207	mp-19395	MnO2	Zn	1.24
208	mvc-15040	Mn13Si2(SbO14)2	Zn	1.24
209	mp-540363	VP2O7	Zn	1.26
210	mvc-10912	CaMnIrO6	Zn	1.26
211	mvc-11834	BaTlCuO4	Zn	1.26
212	mp-19326	MnO2	Zn	1.26
213	mvc-12603	Mg(FeO2)2	Zn	1.27
214	mvc-9418	Fe13Si2(SbO14)2	Zn	1.28
215	mp-1041693	Cr(WO4)2	Zn	1.30
216	mp-1047386	BiO2	Zn	1.30
217	mp-1046192	Sn5(TeO6)3	Zn	1.30
218	mvc-14984	Ca3Co2(RhO6)2	Zn	1.31
219	mvc-11930	Ca3Mn2(GaO5)2	Zn	1.31
220	mp-1044227	BiWO5	Zn	1.31
221	mp-1041585	Re(WO4)2	Zn	1.32
222	mvc-14254	Ca3Fe2(RhO6)2	Zn	1.34
223	mp-1039074	MgBi	Zn	1.34
224	mp-1042189	Ba2Sb3O8	Zn	1.34
225	mp-782692	Mn7O12	Zn	1.34
226	mp-1042656	W3O8	Zn	1.34
227	mp-1221188	NaCa3Fe(SiO3)8	Zn	1.35
228	mvc-12611	CaCr4O8	Zn	1.36
229	mp-32527	V(PO3)4	Zn	1.37
230	mp-1046632	Sr2CoSO3	Zn	1.37
231	mp-1041534	Mo(WO4)2	Zn	1.37
232	mvc-11008	Ba2Fe3O8	Zn	1.37
233	mvc-15204	Ta2Bi2O9	Zn	1.37
234	mvc-11007	CaFeMoO6	Zn	1.38
235	mp-1048779	Mg(BiO3)2	Zn	1.39

236	mvc-13721	Ba2Ni3O8	Zn	1.39
237	mvc-5444	MnO2	Zn	1.41
238	mp-1041470	CrCuO4	Zn	1.42
239	mvc-11883	Ca3Cu6(PO4)8	Zn	1.43
240	mp-1041577	Sn(WO4)2	Zn	1.44
241	mvc-11375	Mg2Mn2(SiO4)3	Zn	1.45
242	mp-1041860	Te(WO4)2	Zn	1.45
243	mvc-12570	Mg(NiO2)4	Zn	1.46
244	mvc-14970	Ti4(FeO4)3	Zn	1.46
245	mp-1045327	Ca(BiO3)2	Zn	1.46
246	mp-1047752	Sb(WO4)2	Zn	1.47
247	mp-1046617	Sr2MnSO3	Zn	1.47
248	mp-777836	Li14Co13O28	Zn	1.47
249	mvc-12565	Mg(CoO2)4	Zn	1.47
250	mvc-14848	CaCu2(P2O7)2	Zn	1.48
251	mvc-14468	MgV6(FeO6)4	Zn	1.48
252	mvc-13642	VF4	Zn	1.48
253	mvc-11924	Mg3Bi2(AsO6)2	Zn	1.49
254	mp-1221467	MoO4	Zn	1.49
255	mvc-13345	Al5(NiO4)3	Zn	1.49
256	mp-1041598	Fe(WO4)2	Zn	1.49
257	mvc-11632	VBiO5	Zn	1.49
258	mp-1043651	BiSbO5	Zn	1.49
259	mvc-15207	Ta2Bi2O9	Zn	1.49
260	mvc-5220	BiO2	Zn	1.49
261	mvc-13126	Ca5Sc2(CoO6)2	Zn	1.50
262	mvc-15035	Ca3Ga2(FeO5)2	Zn	1.50
263	mp-1228752	Al4Cu15	Zn	1.51
264	mp-1045006	Ba2Ti2CuF14	Zn	1.52
265	mp-1043556	SbPO5	Zn	1.53
266	mp-1048924	FePO4	Zn	1.53
267	mvc-10906	Ca2MnNiO6	Zn	1.53
268	mp-1044170	CrPO5	Zn	1.53
269	mp-1048554	Ba2Ni3O7	Zn	1.53
270	mp-1221093	NaCaFe(SiO3)4	Zn	1.54
271	mvc-6353	MnO2	Zn	1.54
272	mp-765928	VF5	Zn	1.55
273	mvc-12258	Ca2Mn2(SiO4)3	Zn	1.57
274	mvc-11096	MoO3	Zn	1.57
275	mvc-14697	SbF5	Zn	1.59
276	mp-1147673	Cu3O4	Zn	1.59
277	mvc-11380	V2CoO7	Zn	1.59
278	mp-1048511	Ba2Mn3O7	Zn	1.59
279	mvc-13581	Al2Fe3(PO5)3	Zn	1.60
280	mvc-11916	Ca2La5Mn7NiO24	Zn	1.60
281	mvc-11865	CaCoSi2O7	Zn	1.61

282	mvc-12807	CaMnFeO5	Zn	1.61
283	mvc-14253	Ca3Mn2O7	Zn	1.62
284	mp-1047617	Co(WO4)2	Zn	1.62
285	mp-687212	Cr(PO3)4	Zn	1.62
286	mvc-14980	CaMn2O5	Zn	1.63
287	mvc-14109	Al4(CoO4)3	Zn	1.63
288	mvc-11181	Al(CuO2)3	Zn	1.64
289	mvc-13490	Bi2O5	Zn	1.65
290	mvc-8434	Cr(GeO3)2	Zn	1.66
291	mvc-14116	Al4(CoO4)3	Zn	1.68
292	mvc-13172	Ba4CaV4Cu2F28	Zn	1.69
293	mp-694636	MnP2O7	Zn	1.69
294	mvc-12050	NiO2	Zn	1.70
295	mp-775128	Fe3Sb(PO4)6	Zn	1.70
296	mp-1042304	Ni(WO4)2	Zn	1.71
297	mp-1043461	NiSbP2O9	Zn	1.71
298	mp-540267	CrP2O7	Zn	1.71
299	mvc-11548	CrO3	Zn	1.72
300	mvc-12893	Al4(NiO4)3	Zn	1.72
301	mp-644514	MnO2	Zn	1.72
302	mvc-11646	BaCo4O7	Zn	1.72
303	mp-1046591	Ba2Tl2Ni3O10	Zn	1.73
304	mvc-11457	WO3	Zn	1.73
305	mvc-15002	Al4(FeO4)3	Zn	1.74
306	mp-769727	Li3(NiO2)4	Zn	1.74
307	mp-1197460	Al4Fe(SiO6)2	Zn	1.74
308	mp-1045817	Ba2CuMo2F14	Zn	1.75
309	mvc-11925	MgBiPO6	Zn	1.75
310	mvc-14924	Al4(FeO4)3	Zn	1.78
311	mp-31998	Mn(PO3)4	Zn	1.79
312	mp-1041572	Bi(WO4)2	Zn	1.79
313	mvc-13536	CrF4	Zn	1.80
314	mp-1042873	Sn(GeO3)2	Zn	1.80
315	mvc-13999	CrO3	Zn	1.81
316	mvc-10979	CaCu2(GeO3)4	Zn	1.82
317	mp-540321	FeP2O7	Zn	1.82
318	mvc-4519	SiNiO4	Zn	1.84
319	mp-1117519	Cr2O5	Zn	1.84
320	mp-1172361	CoSiO4	Zn	1.85
321	mvc-12198	Fe(SiO3)2	Zn	1.85
322	mvc-13059	Ca3Cu6(AsO4)8	Zn	1.86
323	mp-1221542	MnO2	Zn	1.86
324	mp-1048188	Ba2Sn3O7	Zn	1.86
325	mp-769642	Fe(CO3)2	Zn	1.87
326	mvc-12739	CaCu2(GeO3)4	Zn	1.87
327	mvc-12287	Mg2Fe2(SiO4)3	Zn	1.88

328	mp-771678	NaFe2(SiO3)4	Zn	1.89
329	mvc-2990	Ba2TlNi2O7	Zn	1.90
330	mp-770908	CoO2	Zn	1.91
331	mp-1116784	CoO2	Zn	1.92
332	mp-1117500	SnF4	Zn	1.92
333	mvc-12905	FeO2	Zn	1.93
334	mp-766786	VF5	Zn	1.94
335	mp-1041261	Bi3P3O13	Zn	1.94
336	mvc-7342	Si2NiO6	Zn	1.94
337	mvc-1739	Ba2CuSn2F14	Zn	1.96
338	mvc-11848	CaBiAsO6	Zn	1.96
339	mvc-11862	CaCu2(As2O7)2	Zn	1.97
340	mvc-10914	CrP2O7	Zn	1.99
341	mvc-11097	CrO3	Zn	2.00
342	mvc-14138	Al2(FeO3)3	Zn	2.01
343	mp-1048124	Ba2Cr3O8	Zn	2.01
344	mvc-12271	Ca2Fe2(SiO4)3	Zn	2.03
345	mp-1044399	Mn(GeO3)2	Zn	2.03
346	mvc-10933	CaLa2Mn2(FeO6)2	Zn	2.03
347	mp-1042286	Co(SiO3)2	Zn	2.05
348	mp-1042757	CrAs2O7	Zn	2.07
349	mp-1042331	Mn(SiO3)2	Zn	2.08
350	mvc-10920	CaFe2F10	Zn	2.13
351	mvc-12194	Al10(Bi2O9)3	Zn	2.14
352	mp-585256	Co(PO3)4	Zn	2.15
353	mvc-13141	Al4(FeO4)3	Zn	2.17
354	mp-1094572	Mg2Sb	Zn	2.20
355	mp-1044639	Fe(GeO3)2	Zn	2.22
356	mvc-13128	AlFe3F15	Zn	2.22
357	mp-1041062	Fe2P2O9	Zn	2.23
358	mvc-13941	CoF4	Zn	2.26
359	mp-1043444	Ni(GeO3)2	Zn	2.27
360	mvc-8361	Co(GeO3)2	Zn	2.31
361	mp-540262	CoP2O7	Zn	2.33
362	mp-773979	Cr(SO4)2	Zn	2.35
363	mp-1048486	BaNi4O7	Zn	2.37
364	mp-540273	NiP2O7	Zn	2.41
365	mp-1048172	Ba2Mn3O8	Zn	2.45
366	mvc-13181	FeO2	Zn	2.50
367	mvc-13155	Mn3AlF15	Zn	2.62
368	mp-1221594	MnO4	Zn	2.64
369	mvc-12753	CaMn2F10	Zn	2.68
370	mvc-14958	Ba2CaCr2F14	Zn	2.72
371	mp-1018795	Mg2Sn	Zn	2.74
372	mp-1039182	Mg2Bi	Zn	2.80
373	mvc-15217	Bi3(PO5)2	Zn	2.98

374	mp-1094498	Mg5Ti	Zn	3.34
375	mvc-14843	Al(BiO3)3	Zn	4.14
376	mvc-11777	Al(BiO3)3	Zn	4.21
377	mp-1094189	Mg5Sn	Zn	4.73

Supplementary References

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2 Urban, A., Seo, D.-H. & Ceder, G. Computational understanding of Li-ion batteries. *npj Comput. Mater.* **2**, 16002 (2016).

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