Supporting Information for 'Electrochemical Pourbaix diagrams of Mg-Zn alloys from first-principles calculations and experimental thermodynamical data'

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Table S1. Calculated lattice constants, formation energies, and volume per atom of partial results of the high-throughput of Mg-Zn alloys from the Inorganic Crystal Structure Database (ICSD) prototype library[1].

	Lattice constants/ Å			Formation energy/meV	Volume per atom/Å^3	ICSD number	Pearson symbol
	a	b	c				
MgZn	3.189	4.403	5.44	-93.311	18.465	56541	mP4
	10.189	10.189	5.722	-93.009	18.565	78364	tI32
	5.426	10.455	5.426	-93.59	18.341	104584	mP16
	6.44	8.748	5.472	-96.413	18.482	167597	mS16
	5.383	10.624	5.118	-85.932	18.295	57734	oP16
	12.051	4.392	5.562	-91.754	18.401	58358	oP16
	10.203	10.203	5.71	-92.928	18.575	78364	tI32
	5.41	10.436	5.425	-95.148	18.407	104584	mP16
$MgZn_2$	5.217	5.217	5.217	-123.821	16.803	2351	hR6
	5.218	7.396	5.209	-122.623	16.751	2459	oP12
	5.218	7.396	5.209	-122.623	16.751	28383	hP39
	7.378	7.378	7.378	-124.393	16.732	103048	cF24
	5.212	5.212	16.904	-127.764	16.567	104838	hP24
	5.217	5.217	8.57	-130.758	16.832	104897	hP12
	5.222	9.036	8.566	-129.656	16.841	105898	oS24
	7.628	7.628	3.082	-92.481	17.258	151889	hP9
	5.223	5.223	7.401	-123.104	16.824	154731	tI12
	5.216	5.213	7.4	-123.09	16.767	154737	oI12
Mg_2Zn	6.758	6.758	5.272	-72.607	20.065	642	tI12
	6.768	6.768	5.273	-72.417	20.13	30446	tI12
	5.418	5.418	14.23	-69.001	20.096	30713	hP18
	6.736	6.736	5.301	-73.206	20.042	42518	tI12
	4.557	5.982	8.698	-60.529	19.758	44507	mP12
	7.907	7.907	3.255	-70.419	19.581	51974	hP9
	5.326	6.654	6.832	-72.739	20.175	60760	mP12
	7.917	7.917	3.247	-70.239	19.588	70115	hP9
	6.63	13.595	7.837	-69.986	19.621	82148	oI36
	7.829	7.829	6.667	-70.766	19.663	103790	hP18
Mg_7Zn_3	9.458	9.458	9.458	-12.262	21.154	53656	cI40
	9.171	16.434	5.548	-12.777	20.904	87129	oP40
	11.242	10.148	7.574	-31.684	20.135	102983	aP40
	4.515	22.342	3.949	-16.816	19.922	104134	oS20
	5.968	8.327	10.378	308.325	25.785	106290	oS20
	9.073	9.073	5.843	-18.028	20.828	107715	hP20
	11.199	3.5	10.403	13.124	20.342	200243	mS20
	13.709	12.092	10.979	78.974	22.748	300282	oS80
Mg_2Zn_{11}	8.559	8.559	8.559	-60.556	16.079	104898	cP39

Table S2. Formation energies, and volume per atom of partial results of Mg-Zn alloys from the Automatic Flow for Materials Discovery (AFLOW)[2–4].

Index	Mg	Zn	Formation energy/meV	Volume per atom/Å^3	Space group
3	1	1	-74.2991	17.945	P4/mmm
4	1	1	-1.2901	18.87	R-3m
5	2	1	-41.8097	19.8	I4/mmm
6	1	2	-32.5518	17.0367	I4/mmm
7	2	1	-26.4187	19.82	Immm
8	1	2	-28.8995	17.0133	Immm
9	2	1	12.3943	20.3667	P-3m1
10	1	2	21.0862	17.6767	P-3m1
11	3	1	8.299	20.5975	Cmmm
12	1	3	-1.5187	16.7175	Cmmm
13	3	1	-27.4415	20.56	P4/mmm
14	2	2	-18.9114	18.535	P4/nmm
15	1	3	-7.8907	16.57	P4/mmm
16	3	1	-3.7278	20.685	C2/m
17	2	2	-57.6106	18.44	C2/m
18	1	3	-6.8227	16.855	C2/m
19	3	1	-6.158	20.615	Pmmm
20	2	2	-8.8146	18.57	Pmmn
21	1	3	-10.7179	16.83	Pmmm
22	3	1	-7.3123	20.38	I4/mmm
23	2	2	-28.1034	18.3975	I4_{1}/amd
24	1	3	-30.0112	16.475	I4/mmm
25	3	1	-14.2955	20.3675	Pm-3m
26	1	3	-41.2949	16.41	Pm-3m
27	3	1	16.8517	20.9775	R-3m
28	2	2	34.5699	19.2625	R-3m
29	1	3	29.8078	16.995	R-3m
60	1	1	-69.9411	18.12	P4/mmm
61	1	1	-74.8876	17.92	Pm-3m
62	2	1	-2.1197	19.7967	P-3m1
63	1	2	-93.0478	17.0733	P6/mmm
66	2	1	-40.9504	19.79	I4/mmm
67	1	2	-25.5888	17.2667	I4/mmm
68	3	1	33.102	20.6325	R-3m
69	1	3	40.3888	16.8125	R-3m
70	3	1	-25.827	20.43	P4/mmm
71	2	2	-16.4236	18.56	P4/nmm
72	1	3	-7.1789	16.6425	P4/mmm
73	3	1	4.58	20.5825	P2/m
74	2	2	-97.0801	18.5675	Cmcm
75	1	3	-29.2444	17.47	P2/m
76	3	1	-12.15	20.3925	P4/mmm

77	2	2	-5.4359	18.675	P4/nmm
78	1	3	-11.0942	16.9075	P4/mmm
79	3	1	-6.781	20.4175	Immm
80	2	2	-41.7339	18.345	Imma
81	1	3	-29.9829	16.43	I4/mmm
82	3	1	-15.0268	20.4175	P4/mmm
83	1	3	-40.3372	16.4925	P4/mmm
84	3	1	13.8905	20.13	Fm-3m
85	2	2	26.6679	17.9275	Fd-3m
86	1	3	1.8878	16.3725	Fm-3m
116	1	1	-11.0986	18.67	P-6m2
118	3	1	-4.8445	20.51	Pmm2
119	2	2	-6.8886	18.565	Pmmn
120	2	2	-80.8119	18.0575	Pmma
121	1	3	-17.1749	16.6125	Pmm2
122	3	1	-10.7923	20.645	Imm2
124	1	3	-9.9304	16.6075	Imm2
125	3	1	1.5405	20.76	P-6m2
126	2	2	16.7341	18.9325	P-3m1
127	1	3	19.4561	16.8475	P-6m2
128	5	1	-2.9818	21.27	Cm
129	2	4	-29.5012	17.2033	C2/m
130	2	4	-39.0035	16.92	C2/m
131	2	4	-12.7673	17.265	C2/m
132	1	5	-0.6669	16.08	Cm
133	4	2	-7.0604	20.0117	Cm
134	4	2	-6.3499	20.045	C2/m
135	4	2	-23.5509	19.8783	C2/m
136	3	3	-3.2149	18.6233	Cm
137	4	2	-37.6626	19.6067	C2/m
138	3	3	-40.7794	18.3783	Cm
139	3	3	-36.6174	18.4383	Cm
140	2	4	-9.8587	17.3283	Cm
141	5	1	2.0155	21.2217	Amm2
142	2	4	17.487	17.5983	Cmcm
143	2	4	-43.5367	16.9533	Cmcm
145	1	5	-0.6459	16.05	Amm2
147	4	2	3.5044	20.16	Cmcm
150	4	2	-29.0362	19.7033	Cmcm
178	8	4	239.2978	21.9525	P6_{3}/mmc
179	4	8	-130.638	16.8258	P6_{3}/mmc
180	12	4	-40.2023	21.1913	Pnma
181	4	12	-15.7086	16.6425	Pnma
182	2	4	-123.912	16.7383	Fd-3m
183	4	2	231.8784	21.84	Fd-3m
184	6	2	3.4536	20.5025	Pm-3n
185	2	6	22.3577	17.2425	Pm-3n
186	6	2	-35.0873	20.1475	P6_{3}/mmc
187	2	6	-57.3641	16.3113	P6_{3}/mmc

188	4	2	-24.7299	19.7117	Cmcm
189	2	4	-40.7672	17.1117	Cmcm
190	2	1	12.6533	20.4	P-3m1
191	1	2	172.7258	20.3933	P-3m1
192	2	2	53.7599	19.3825	Cmcm
193	2	2	-96.2261	18.5175	Cmcm
194	2	2	-96.3534	18.37	Cmcm
195	4	4	-21.6925	18.81	P2_{1}3
196	2	2	-18.8119	18.5975	P4/nmm
197	2	2	-18.6579	18.6325	P4/nmm
198	12	12	-52.9004	18.5579	Pbcm
201	1	1	192.0769	21.885	Fm-3m
202	4	1	266.0914	24.142	I4/mmm
203	1	4	6.3112	17.494	I4/mmm
204	5	1	257.1268	24.695	P6/mmm
205	1	5	-7.4907	16.8017	P6/mmm
208	6	3	-70.8162	19.6522	P-62m
209	3	6	107.6115	19.2411	P-62m
210	4	8	-42.4305	17.1267	Pnma
211	8	4	-60.4917	19.68	Pnma
216	2	1	127.2326	19.8967	P6/mmm
217	1	2	-93.6202	17.09	P6/mmm
218	1	1	556.2019	30.23	F-43m
219	2	2	149.3051	20.2975	P6_{3}mc
220	2	2	40.0044	21.0825	P6_{3}/mmc
221	2	2	-7.6999	18.7825	P6_{3}/mmc
222	6	10	50.1522	18.8325	P6_{3}/mcm
223	10	6	-65.8774	19.7719	P6_{3}/mcm
230	2	4	172.4075	19.5667	I4/mcm
231	4	2	-73.0552	19.9283	I4/mcm
232	2	1	-41.9431	19.8667	I4/mmm
233	1	2	-32.7998	17.15	I4/mmm
234	4	2	-73.1132	19.9633	I4/mcm
235	2	4	172.512	19.5367	I4/mcm
238	18	6	-22.4743	20.2662	P6_{3}/mmc
239	6	18	-46.3796	16.3829	P6_{3}/mmc
242	18	6	-13.2561	20.2787	Pmmn
243	6	18	-37.8921	16.4671	Pmmn
244	4	12	-48.3597	16.4475	P6_{3}/mmc
245	12	4	-26.709	20.2869	P6_{3}/mmc
246	4	2	127.1988	20.0467	P6/mmm
247	2	4	-91.2417	17.325	P6/mmm
248	2	4	46.3182	18.9967	I4_{1}/amd
249	4	2	14.1663	20.7383	I4_{1}/amd
252	5	1	159.0165	22.7217	F-43m
253	1	5	-14.0665	16.2167	F-43m
254	10	6	-55.8173	19.6581	I4/mcm
255	6	10	27.8317	18.065	Fmmm
256	4	4	28.6146	19.345	Pnma

257	4	2	-26.5416	19.7067	Immm
258	2	4	-32.4165	17.2267	Immm
259	2	3	11.1447	18.164	R-3m
260	3	2	5.3535	19.802	R-3m
261	16	8	-53.3133	19.8967	Fd-3m
262	8	16	119.4445	18.7079	Fd-3m
263	4	3	-23.5354	19.0771	I4/mmm
264	3	4	-14.9968	17.88	I4/mmm
267	4	2	-26.5416	19.7067	Immm
268	2	4	-32.4165	17.2267	Immm
269	1	2	-92.9428	17.2133	P6/mmm
270	2	1	-2.5914	19.9433	P-3m1
271	6	2	-34.7852	20.1325	P6_{3}/mmc
272	2	6	-60.1792	16.5437	Cmcm
273	2	4	19.4263	17.2967	P6_{3}/mmc
274	4	2	-47.2879	19.5483	P6_{3}/mmc
275	2	4	19.4283	17.31	P6_{3}/mmc
276	4	2	-47.2769	19.5983	P6_{3}/mmc
277	2	6	-64.5689	16.6225	Pmmn
278	6	2	-26.9137	20.1762	Pmmn
279	2	6	-37.4568	16.5675	I4/mmm
280	6	2	-11.7262	20.3388	I4/mmm
281	8	4	44.7777	22.6425	Fm-3m
282	4	8	391.1893	23.1975	Pa-3
283	4	8	43.9917	18.8092	I4_{1}/amd
284	8	4	18.3892	20.75	Imma
285	4	1	71.5694	20.75	I4/m
286	1	4	-167.741	20.75	I4/m
287	2	1	-41.2061	19.5667	I4/mmm
288	1	2	-30.9935	17.1767	I4/mmm
289	3	1	336.9872	33.9475	Pm-3m
290	1	3	674.9231	40.0575	Pm-3m
291	2	2	-71.7069	18.125	P4/mmm
292	2	2	-74.3829	17.9875	P4/mmm
309	7	1	15.5919	21.8525	Fm-3m
310	1	7	8.5862	15.93	Fm-3m
311	1	8	-0.2213	15.7144	I4/mmm
312	8	1	10.7381	21.8489	I4/mmm
313	5	4	-14.5709	18.6478	I4/mmm
314	4	5	-37.3722	17.9222	I4/mmm
315	16	8	234.2803	21.9788	P6_{3}/mmc
316	8	16	-127.879	16.5933	P6_{3}/mmc
359	10	8	-39.2489	18.9833	P6_{3}/mcm
360	8	10	-6.0862	18.115	P6_{3}/mcm
363	4	3	-66.1374	18.9014	P6/mmm
364	3	4	99.5963	19.6143	P6/mmm
365	4	6	88.2006	19.6143	Fdd2
366	6	4	167.9708	19.6143	Fdd2
371	2	3	98.5919	19.952	P-3m1

372	3	2	-40.1521	20.266	P-3m1
373	4	16	15.6652	17.524	I-43m
374	16	4	165.141	23.569	I-43m
375	5	3	-43.1044	19.2838	Cmmm
376	3	5	-40.3118	17.36	Cmmm
381	4	8	-42.6608	16.9567	I4_{1}/amd
382	8	4	-19.8901	19.5908	I4_{1}/amd
389	1	2	193.9075	21.89	P4/mmm
390	2	1	44.6616	22.4033	P4/mmm
405	2	2	26.9189	18.165	I4_{1}/amd
406	2	2	-37.0056	19.605	R-3m
407	4	4	131.3038	19.8762	P6_{3}/mmc
408	4	4	-36.2757	19.015	P6_{3}/mmc
447	2	2	-74.4029	18.2675	P2_{1}/m
448	2	2	-80.2654	18.035	Pmma
471	2	6	-13.2572	16.5162	Cmcm
472	6	2	-4.1122	20.5	Cmcm
473	1	5	-19.632	15.89	P-62m
474	5	1	-2.3307	21.145	P-62m
475	4	2	-5.6232	19.9933	C2/m
476	2	4	-31.2412	17.2167	C2/m
477	1	5	8.2926	16.035	P4/mmm
478	5	1	-11.0157	21.3817	P4/mmm
479	5	1	1.6922	21.1583	Cmmm
480	1	5	-16.7367	16.0433	Cmmm
521	6	3	-70.6545	19.5667	P-62m
522	3	6	58.7713	17.7033	P-62m
531	1	3	-40.3372	16.53	Pm-3m
532	3	1	-13.9323	20.4075	Pm-3m
537	6	6	-37.3659	19.3642	R-3m
538	6	6	26.4409	18.0258	R-3m
539	2	4	-42.4902	16.98	C2/m
540	4	2	-40.4962	19.6217	C2/m
541	1	3	-29.1932	16.595	I4/mmm
542	3	1	-6.0335	20.6125	Immm
543	2	2	-41.4496	18.41	Imma
545	2	1	-2.1444	20.1367	P-3m1
547	1	2	-32.5165	17.1133	I4/mmm
548	2	1	-41.9221	19.7233	I4/mmm
551	1	3	-10.0737	16.5475	Imm2
553	6	18	-60.2406	16.9546	P6_{3}/mmc
554	18	6	-42.9881	20.6604	P6_{3}cm
583	2	1	43.2079	22.65	Fm-3m
584	1	2	240.6392	21.14	Fm-3m
585	2	6	106.7694	18.175	P6_{3}/mmc
586	6	2	-16.201	20.815	P6_{3}/mmc
590	6	33	-60.6008	16.0651	Pm-3
592	20	35	-126.791	16.8251	C2/m

Figure S1. (a) Theoretical bound conditions of corrosion, immunity and passivation of the Mg:Zn = 10:1 system at 298 K; (b) Theoretical conditions of corrosion, immunity and passivation of the Mg:Zn = 10:1 system in Cl-containing solutions at 298 K; (c) Theoretical conditions of corrosion, immunity and passivation of the Mg:Zn = 1:10 system at 298 K; (d) Theoretical conditions of corrosion, immunity and passivation of the Mg:Zn = 1:10 system in Cl-containing solutions at 298 K.

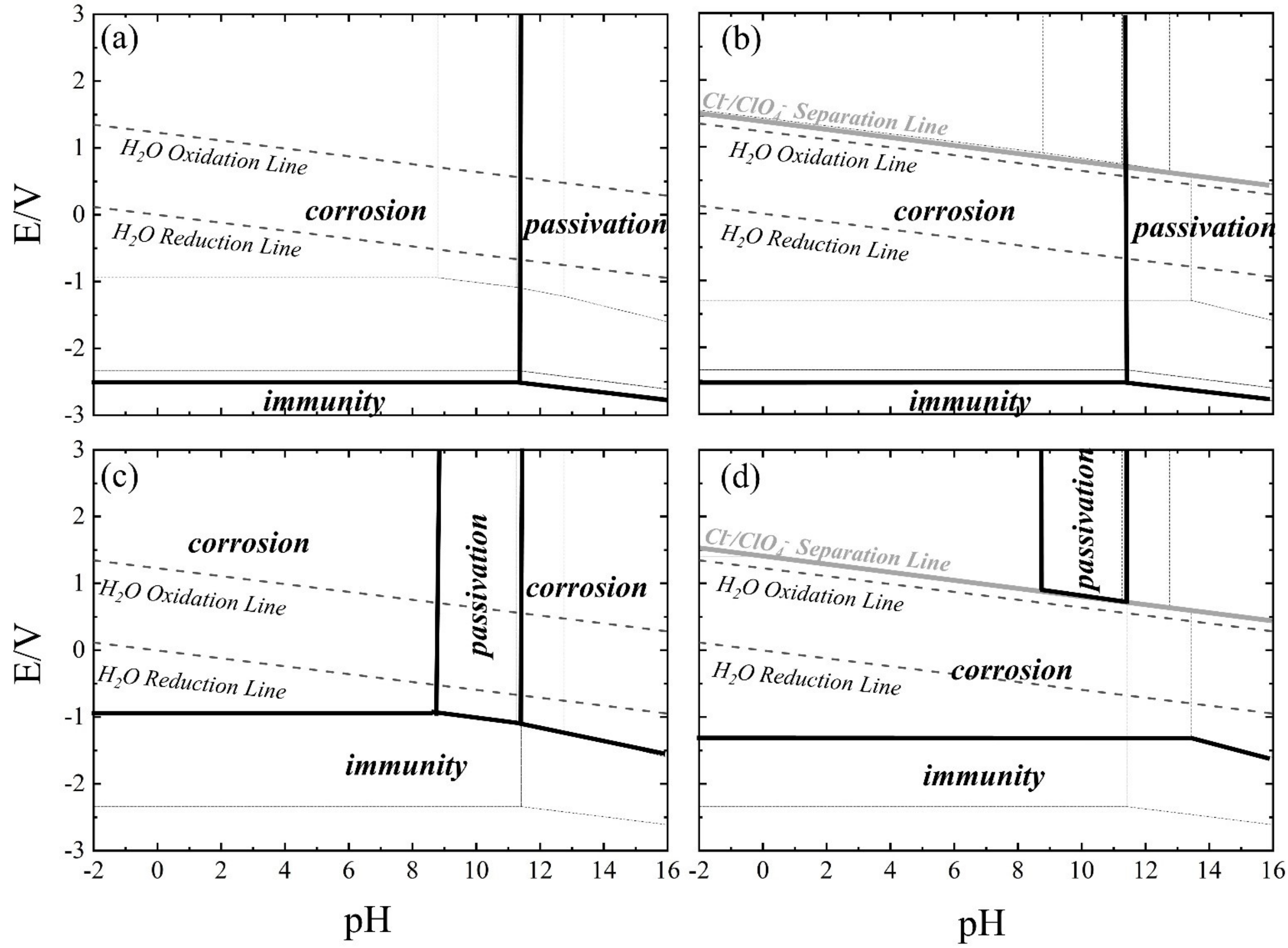
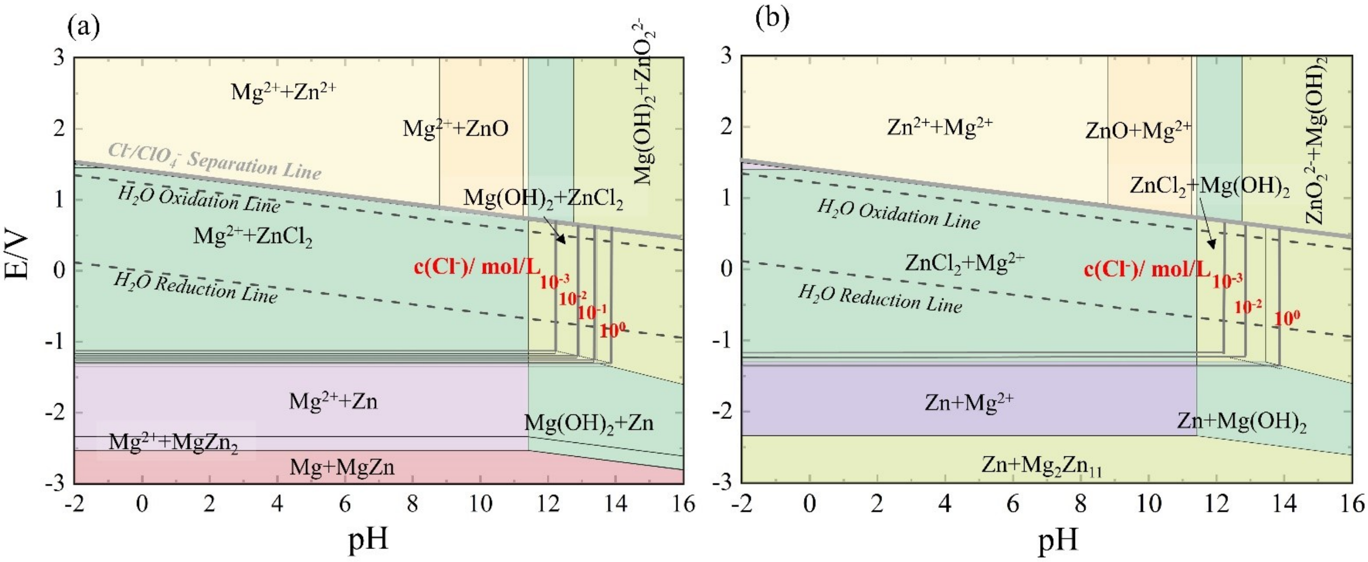


Figure S2. (a) Pourbaix diagram of the Mg: Zn = 10:1 system in Cl-containing solution at 298 K; (d) Pourbaix diagram of the Mg: Zn = 1:10 system in Cl-containing solution at 298 K. The different concentrations of Cl- and their corresponding stable domains are marked in the diagrams.



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