

Supporting Information

A Practical Perspective to the Potential of Rechargeable Mg Batteries

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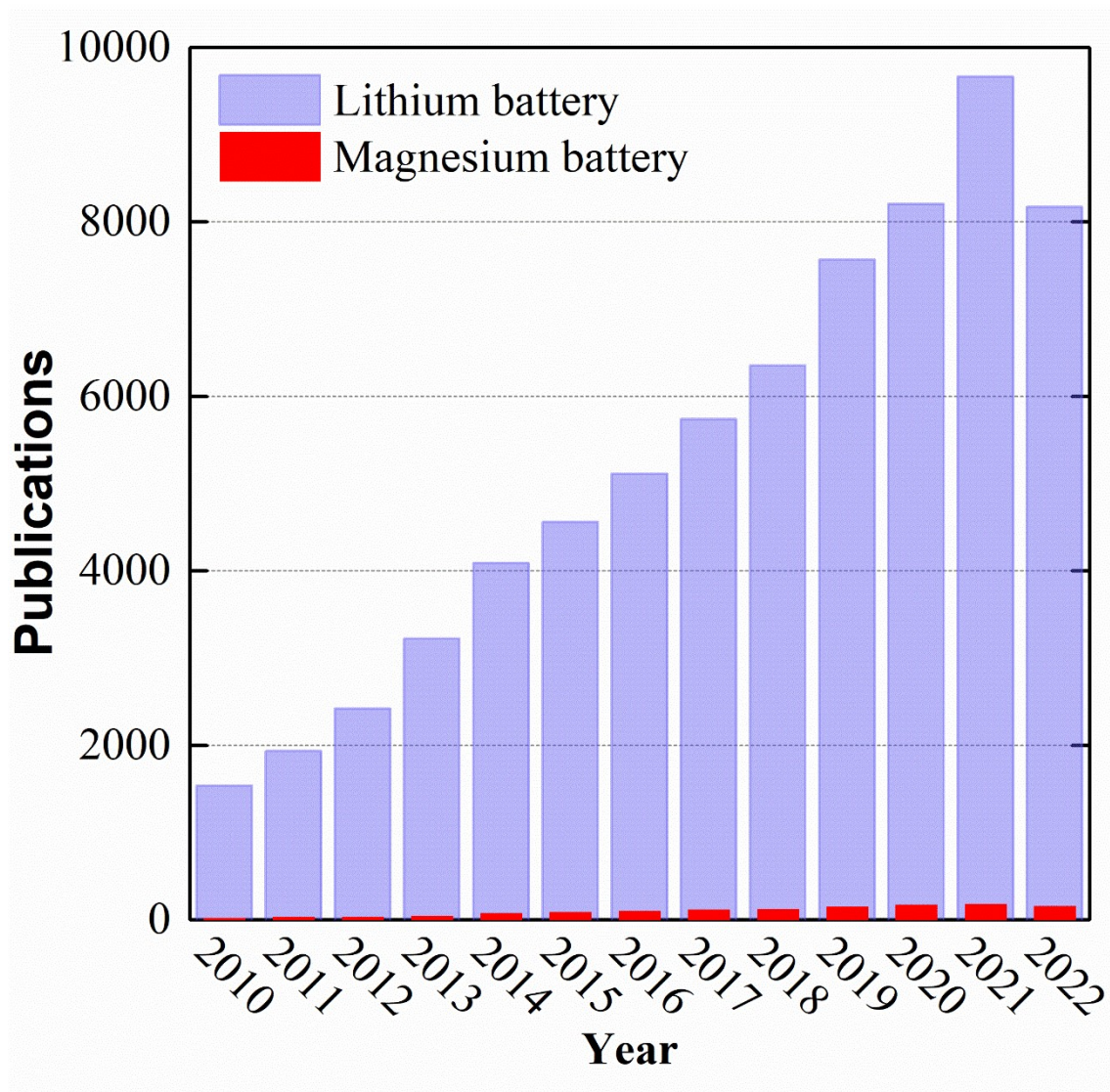


Figure SI. 1 Number of publications per year, including the words “lithium batteries” or “magnesium batteries” in the titles, appeared in the literature during the last two decades. The data collected is based on the Web of Science.

Experimental: High purity Mg metal foil (99.9%, 100 μm) was provided by Gelon LIB group, Chevrel Phase was provided by American NEI Corp. (1 kg) and pouch cell cathodes were processed in a pilot plant line using CP/carbon black (C45)/PVDF (90:5:5) reaching 11.8 $\text{mg}_{\text{CP}}/\text{cm}^2$ loading (1.6 mAh/cm^2) on both sides of nickel current collector (Gelon LIB group, 20 μm) while coin cell cathodes with nickel current collector were produced in the laboratory setting by doctor blade technique reaching 3.5 $\text{mg}_{\text{CP}}/\text{cm}^2$ loading. Pouch cell prototypes consisted of five pure magnesium metal foil anodes (44 x 61 mm), four double-sided cathodes (43 x 60 mm) stacked with double layer polyolefin-based separator in between, unless indicated otherwise. 2025 type coin cells consisted of one layer of pure magnesium metal foil anode, single-side coated cathode and a layer of Whatman glass fiber (GF/F) in between. The assembly of coin cells were done in a high-purity Ar (99.999%) filled glovebox (MBraun, Germany) under ideal conditions ($\text{O}_2 < 1$

ppm, $H_2O < 1$ ppm) whereas pouch cells were assembled in a dry room (dew point $-50^{\circ}C$) using standard pouch cell packaging foil (Targray) and nickel tabs (Gelon LIB group). The assembly of the scaled-up conventional multilayer RMB pouch cell is adapted for magnesium battery system from the Li-ion pouch cell assembly know-how and experience. The pouch cells were sealed under vacuum conditions in the above-mentioned glovebox with APC. Electrolyte amounts used were 100 μ L in case of coin cell and 3 mL in pouch cell unless specified. Prior to cycle life test, a 10 cycle activation protocol was applied.

Calculations: The calculation spreadsheet images are given for the energy density and mass distribution values represented in Table 1 of the article. The component and value changes in each battery is highlighted for clarity.

1. Assembled Conventional RMB Coin Cell

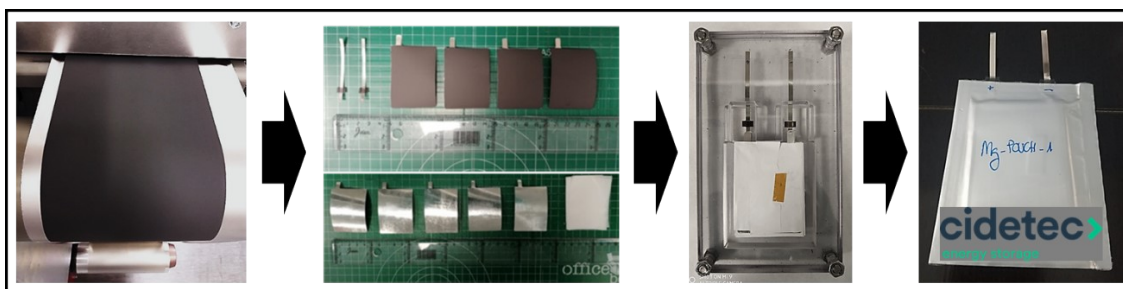
CP	90	
C45	5	
Binder	5	
	Mass (mg)	(%)
CP Cathode x1 (3.5 mg/cm ²)	8.416	3.98
Current Coll. (Ni 20 μ m)	32.000	15.14
APC Electrolyte (100 μ l)	94.850	44.88
Separator GF/F	38.458	18.20
Mg anode (100 μ m)	37.614	17.80
Total	211.338	100.00
Specific capacity (mAh/gCP)	61.6	
Specific capacity (mAh/gEI)	55.44	
Loading (mgCP/cm ²)	3.5	
Capacity (mAh/cm ²)	0.2156	
Capacity Mg (100 μ m, 2,1642cm ²)	99.72	
Excess of Mg (1 to 1)	213.71 times	
Electrolyte Vol./Capacity (mAh)	214.32 μ l/mAh	
Electrolyte Vol./mg(CP)	13.20 μ l/mg	
Ni CC/Cathode Total Mass	79.18 %	
Wh (experimental)	0.00023716	
Wh/kg	2.37	

2. Assembled Conventional RMB Pouch Cell

CP	90	
C45	5	
Binder	5	
	Mass (mg)	(%)
CP Cathode x4 (11.8 mg/cm ²)	2706.133	27.27
Current Coll. (Ni 20 um)	1525.922	15.38
APC Electrolyte (3000 ul)	2845.500	28.67
Separator POx2	513.555	5.18
Mg anode x5 (100 um)	2332.396	23.50
Total	9923.506	100.00
Specific capacity (mAh/gCP)	64.66	
Specific capacity (mAh/gEI)	58.194	
Loading (mgCP/cm ²)	11.8	
Capacity (mAh/cm ²)	0.762988	
Capacity Mg (100 um, 44x61cm ² Mg)	1028.78	
Excess of Mg (5 to 4)	32.66	times
Electrolyte Vol./Capacity	19.05	ul/mAh
Electrolyte Vol./mg(CP)	1.23	ul/mg
Ni CC/Cathode Total Mass	36.06	%
Wh (experimental)	0.18199497	
Wh/kg	18.34	

Pouch cell assembly steps:

CP cathode cutting from the roll (11.8 mg_{CP}/cm² loading), Mg metal anode, PO-based separator (double layer unless specified) cutting and tab preparation. Assembly of the inner cell and final packaging.



3. Modified RMB Pouch Cell + Al + Mg - fluoro-organo borate/DME electrolyte solution (Estimated)

CP	90	
C45	5	
Binder	5	
	Mass (mg)	(%)
CP Cathode x4 (11.8 mg/cm ²)	2706.133	29.40
Current Coll. (Al 12 um)	277.527	3.02
Borate Electrolyte (3000 ul)	3375.000	36.67
Separator POx2	513.555	5.58
Mg anode x5 (100 um)	2332.396	25.34
Total	9204.612	100.00
Specific capacity (mAh/gCP)	64.66	
Specific capacity (mAh/gEI)	58.194	
Loading (mgCP/cm ²)	11.8	
Capacity (mAh/cm ²)	0.762988	
Capacity Mg (100 um, 44x61cm ² Mg)	1028.78 mAh	
Excess of Mg (5 to 4)	32.66 times	
Electrolyte Vol./Capacity	19.05 ul/mAh	
Electrolyte Vol./mg(CP)	1.23 ul/mg	
Al CC/Cathode Total Mass	9.30 %	
Wh (experimental)	0.18199497	
Wh/kg	19.77	

4. Modified RMB Pouch Cell + Al + VS₄ cathode + Optimized Electrolyte solution (Estimated)

VS4	90	
C45	5	
Binder	5	
	Mass (mg)	(%)
VS4 Cathode x4 (11.8 mg/cm ²)	2706.133	33.80
Current Coll. (Al 12 um)	277.527	3.47
Borate Electrolyte (1935 ul)	2176.875	27.19
Separator POx2	513.555	6.41
Mg anode x5 (100 um)	2332.396	29.13
Total	8006.487	100.00
Specific capacity (mAh/gVS4)	300	
Specific capacity (mAh/gEI)	270	
Loading (mgVS4/cm ²)	11.8	
Capacity (mAh/cm ²)	3.54	
Capacity Mg (100 um, 44x61cm ² Mg)	1028.78	
Excess of Mg (5 to 4)	7.04 times	
Electrolyte Vol./Capacity	2.65 ul/mAh	
Electrolyte Vol./mg(VS4)	0.79 ul/mg	
Al CC/Cathode Total Mass	9.30 %	
Wh (estimated)	0.94504023	
Wh/kg	118.03	

5. Advanced RMB Pouch Cell + Al + VS₄ cathode + Optimized Electrolyte solution + AZ31 Mg alloy thin foil anode (Estimated)

VS4	90	
C45	5	
Binder	5	
	Mass (mg)	(%)
VS4 Cathode x4 (11.8 mg/cm ²)	2706.133	44.89
Current Coll. (Al 12 um)	277.527	4.60
Borate Electrolyte (1935 ul)	2176.875	36.11
Separator POx1	256.778	4.26
AZ31 Alloy anode x5 (25 um)	610.872	10.13
Total	6028.185	100.00
Specific capacity (mAh/gVS4)	300	
Specific capacity (mAh/gEI)	270	
Loading (mgVS4/cm ²)	11.8	
Capacity (mAh/cm ²)	3.54	
Capacity AZ31 (25 um, 44x61cm ²)	246.91	
Excess of Mg (5 to 4)	1.69 times	
Electrolyte Vol./Capacity	2.65 ul/mAh	
Electrolyte Vol./mg(VS4)	0.79 ul/mg	
Al CC/Cathode Total Mass	9.30 %	
Wh (estimated)	0.94504023	
Wh/kg	156.77	

6. Reference LFP – Graphite system (Estimated)

LFP	90	
C45	5	
Binder	5	
	Mass (mg)	(%)
LFP Cathode x4 (11.8 mg/cm ²)	2706.13	33.52
Current Coll. (Al 12 um)	277.527031	3.44
Carbonate Electrolyte (1935 ul)	2418.75	29.96
Separator POx1	513.555	6.36
Graphite (90%)	1389.14	17.21
Current Coll. (Cu 10 um)	767.48	9.51
Total	8072.58203	100.00
Specific capacity (mAh/gLFP)	140	
Specific capacity (mAh/gEI)	126	
Loading (mgLFP/cm ²)	11.8	
Capacity (mAh/cm ²)	1.65	
Capacity Graphite	300	
Excess of Graphite	1.1 times	
Electrolyte Vol./Capacity	6.00 ul/mAh	
Electrolyte Vol./mg(LFP)	0.79 ul/mg	
Al CC/Cathode Total Mass	9.30 %	
Wh (estimated)	1.0911	
Wh/kg	135.16	