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FUNCTIONAL MATERIALS FOR GREEN ENERGY AND ENVIRONMENT

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Supporting Information

Practical Energy Densities, Cost, and Technical Challenges for Magnesium-Sulfur Batteries

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Table S1. A summary of currently reported Mg/S batteries.

Cathode material	Sulfur contents/ loading	Separator Type	Anode material	Electrolyte	Cell type	First Discharge Potential (V)	Coulombic efficiency (%)	current rate/ number of cycles Capacity/(mAh g^{-1})	References
S@carbon black on carbon substrate	61 wt%	No data	Mg foil	$[Mg_2(\mu\text{-}Cl)_3{\cdot}6THF]c$ $[HMDSAlCl_3]$/THF	Coin	0.89	≈ 95	no data/2/394	1
CMK3/S on Al foil	70 wt%	No data	Mg disc	0.3 M $Mg(TFSI)_2$/ DME-diglyme	Coin	0.5	No data	C/30/4/100	2
S/CMK on Inconel 625 collectors	55 wt%	Glass fiber	Pressed Mg powder/carbon black (4:1 wt.)	1.2 M $(HMDS)_2Mg$–$2AlCl_3$–$MgCl_2$ in tetraglyme or diglyme; 1.2 M $(HMDS)_2Mg$–$2AlCl_3$–$MgCl_2$ in diglyme or tetraglyme/PP14TFSI	Swagelok type	No data	≈ 100	0.01 C/20 /150/ with PVDF, diglyme 0.01 C/20 /200 with CMC, diglyme 0.01 C/20/250 with PVDF, tetraglyme 0.01 C/20/260 with CMC, tetraglyme	3
ACC-S	15 wt% 0.5 mg cm^{-2}	Glass fiber	Mg foil	0.1 M $(HMDS)_2Mg$–$2AlCl_3$ + 1 M LiTFSI	Swagelok type	~ 1.7	≈ 92	0.03 C/30/1000	4

S/bis (undec-10-enoyloxymethylbenzo)-18-crown-6-ether (BUMB18C6); sulfur-oxybis(2, 1-ethanediyloxy-2,1-ethanediyl) ester (UOEE) on SS	No data	Celgard 2500	Mg plate	0.5 M $Mg(TFSA)_2$ in triglyme or acetonitrile	Coin	No data	No data	0.01 C/10/23 and 0.01C/10/ 68.1	[5]
S–N-doped graphene on Al foil	50 wt%	Celgard 2400	Mg disc	$Mg(THF)_6][AlCl_4]_2$/ PYR14(TFSI) in THF (salt)	Coin	No data	No data	0.01 C/20/40	[6]
rGo–S on Inconel 625 current collector	49 wt%	Celgard 2400	Pressed Mg powder/ carbon black	$(HMDS)_2Mg–2AlCl_3–MgCl_2$ in tetraglyme	Swagelok type	1.67	≈100	0.01 C/50/236	[7]
CNF–S	50 wt%	Carbon nanofiber-coated glass fiber	Mg foil	3.6 M $(HMDS)_2$ $Mg–2AlCl_3–MgCl_2$ in tetraglyme	Coin	No data	≈ 85	0.01 C/20/800	[8]
S–carbon on Al/C	1 mg cm^{-2}	Glass fiber	Pressed Mg/graphite anode	HMDSMgCl	Swagelok type	No data	≈ 100	0.1 C/100/30	[9]

S–CNT on Cu foil	49 wt% 1.5 mg cm^{-2}	Glass fiber	Mg foil	OMBB 0.5 M $[Mg_4Cl_6(DME)_6]^{2+}$ $[B(HFP)^4]^-$–2 $B(HFP)_3$–$MgCl_2$	Coin	1.15	≈ 100	0.1 C/100/1000	10
ACC–S	1.5 mg cm^{-2}	Glass fiber	Mg disc	1 M $Mg(TFSI)_2$–$MgCl_2$ in DME	Swagelok type	No data	93	0.01 C/100/600	11
SGDY on Al foil	1 mg cm^{-2}	Glass fiber	Mg disc	$(PhMgCl)_2$–$AlCl_3$ + LiCl in THF	Coin	0.87	≈ 100	0.1 C/100/800	12
S/C on SS/Cu	No data	PE membrane	Mg ribbon	0.4 M $(PhMgCl)_2$–$AlCl_3$ + LiCl in THF	Coin	1.65	≈ 100	0.005 C/40/300	13
Graphite/S–multiwalled CNT; on Al foil	85 wt% 0.7 mg cm^{-2}	Glass fiber	Mg foil	0.4 M $Mg(TFSI)_2$–$MgCl_2$ (1:1) in tetraglyme:1,3-dioxolane (DOL) (1:1)	Pouch	0.87	No data	C/60/4/400	14
S/C composite on Cu foil	85 wt%	Glass fiber	Mg foil	BCM (0.5 M THFPB + 0.05 M MgF2 in DME)	Coin	1.1	≈ 100	0.03 C/30/900	15
S/CMK- on SS	1 mg cm^{-2}	Glass fiber	Mg foil	0.8 M $Mg(B(hfip)_4)_2$ in diglyme:tetraglyme (1:1)	Swagelok type	1.4	≈ 100	0.1 C/100/200	16
S-ACC on SS; S/CMK-3 on SS	1 mg cm^{-2}	Glass fiber	Mg disc	$Mg(TFSI)_2$ in DME	Swagelok type	1.25	≈ 100	0.01 C /20/668 0.01 C /3/400	17

Carbon cloth/S	1. mg cm^{-2}	Glass fiber	Mg foil	$Mg(TFSI)_2$–$MgCl_2$ in DME	No data	No data	No data	No data	[18]
S/rGO on N, S dual doped carbon cloth	1 mg cm^{-2}	Activated CNF coated	Mg disc	$(HMDS)_2Mg$–$2AlCl_3$–$MgCl_2$ in tetraglyme	No data	1.45	≈ 93	0.01 C/40/388	[19]
S@MC on Cu foil	64.7 wt%	PE membrane	Mg metal	0.4 M $(PhMgCl)_2$–$AlCl_3$ + 1 M LiCl/THF	Coin	No data	≈ 100	0.1 C/200/368.8	[20]
MOF-S on SS/Mo foil	1 mg cm^{-2}	Glass fiber	Mg foil	$(HMDS)_2Mg$–$2AlCl_3$ with LiTFSI additive	Coin	1.5	No data	0.1 C/200/400	[21]
S-ACC on SS	1.2 mg cm^{-2}	Glass fiber	Mg foil	$Mg[B(hfip)_4]_2$ in DME	Swagelok type	1.68	≈ 100	0.1 C/100 /200	[22]
MgS_8@G-CNT	0.7 mg cm^{-2}	No data	Mg metal	YCl_3–$MgCl_2$ in *N*-methyl-(*N*-butyl)pyrrolidinium bis(trifluoromethanesulfonyl) imide/diglyme (1/1, v/v)	Coin	1.2	98.7	0.04 C/50/900	[23]
S@microporous carbon on Cu foil	55 wt%	PE separator	Mg ribbon	$Mg(CF_3SO_3)_2$–$AlCl_3$ in THF and tetraglyme	Coin	No data	≈ 90	0.05 C/50/400	[24]
S/C	0.35 mg cm^{-2}	Glass fiber	Mg foil	$[Mg(DG)_2][HMDSAlCl_3]_2$	Coin	No data	No data	83 mA g^{-1} /100/400	[25]

Pure sulfur on Ni film	48.8 wt%	Glass Fiber	Mg foil	$MgCl_2$/EnPS	Coin	No data	No data	0.05C/1/400	26
S/C	1 mg cm^{-2}	No data	Mg disk	$MgTFSI_2$/ $MgCl_2$ in DME	Swagelok cells	~ 1.5	No data	100 mAg^{-1} /3/800	27
Sulfur@microporous carbon	41.3 wt%	PE membrane	Mg foil	0.4 mol L^{-1} $(PhMgCl)_2$-$AlCl_3$/THF	Coin	1.3	~ 70%	0.006 C/50/224	28
S/C	No data	No data	Mg foil	0.5 M $Mg(BH_4)_2$/1.0 M THFPB-DGM	Coin	No data	No data	50 mA g^{-1} /30/526	29
Pure sulfur on Al foil	3.0 mg cm^{-2}	CuNWs-GN/PI/LLZO	Mg foil	$B(HFP)_3$, $MgCl_2$ and Mg powders in DME solvent	Coin	No data	No data	100 mA g^{-1}/25/ 915.3	30
C/S on Cu/Al	0.9 mg cm^{-2}	Glass fiber	Mg foil	TFSI based HFIP–Cl based HFIP based	Swagelok type	1.1	No data	No data	31
ACC/S	10 wt.%	Glass fiber	Mg_3Bi_2-C alloy	$Mg(TFSI)_2$/DME	Coin	1.3	No data	C/2/30/400	32
Pure sulfur on carbon paper	0.1 mg cm^{-2}	TiS_2@separator	Mg foil	0.5 M $[Mg(DG)_2][(HMDSAlCl_3)]_2$/DG electrolyte	Coin	1.5	No data	83 mA g^{-1}/30/900	33
Pure sulfur on Cu foil	0.12 mg cm^{-2}	Glass fiber	Mg disk	$Mg(TFSI)_2/MgCl_2$/DME	Coin	1.1	No data	0.1 C/50/600	34
Pure sulfur	No data	Glass fiber	Mg foil	Mg-HMDS-LiTFSI	Coin	~ 1.45	No data	1 C/1/875	35

S/NC on Al foil	0.5 mg cm-$^{-2}$	Polypropy lene	Mg foil	$Mg[B(hfip)_4]_2$/3DME	Swagelok type	1.4	≈ 99	C/50/50/228	36
S_8 on Cu or Al foil	1.2 mg cm$^{−2}$	Glass fiber	Mg metal	Boron-centered anion-based magnesium electrolytes	Coin	No data	No data	C/50/15/550	37
S/CMK3	~2.0 mg cm^{-2}	Glass fiber	Mg disc	OMBB electrolyte	Coin	No data	≈ 99	0.1 C/30/≈1000	38
Sulfurated Poly(acrylonitrile)on a graphite foil	0.6 mg cm^{-2}	Glass fiber	Pressed Mg powde	$Mg[BH_4]_2$ /$Li[BH_4]$ solutions in diglyme	Swagelok / Coin	No data	> 99.8%	0.1 C/100/--	39
VN/60S on Mo foil	60 wt %	Glass fiber	Mg disk	$[Mg_2(\mu\text{-}Cl)_2(DME)_4]^{2+}$ and $[(CF_3SO_3)AlCl_3]^-$	Coin	No data	99.4%	200 mAg^{-1}/20/844	40
MesoCo@C-S	40 wt %	Glass fiber	Mg metal	MMAC-DME	Coin	1.55	90%	0.2C/200/ 280	41
ACC-S	1 mg cm^{-2}	No data	Mg metal	$MgTFSI_2/MgCl_2$ in DME	Coin	No data	No data	0 .1 C/1/396	42

Table S2. Density (g cm^{-3}) of materials in Mg/S cell.

Materials	density
Mg metal	1.738
Sulfur	2.07
Carbon nanotube	2.1 [43, 44]
PVDF	1.78
Super-P	1.9 [44]
Carbon coated Al foil (MTI corp.)	$4.37*10^{-3}$ g cm^{-2}
OMBB electrolyte[a]	1
Solid-state electrolyte (SSE)[b]	1.821
DME	0.87
Celgard 2500	0.946
Al laminated film	1.75
Ethylene carbonate (EC)	1.321 (Sigma-Aldrich)
Propylene carbonate (PC)	1.204 (Sigma-Aldrich)
PVDF-HFP	1.77 (Sigma-Aldrich)
$MgAl_2O_4$	3.64 (Sigma-Aldrich)

(a. The main composite of OMBB electrolyte is 0.5 M $[Mg_4Cl_6(DME)_6][B(HFP)_4]_2$ in DME. The density is approximated at 1 g cm^{-3}. The electrolyte composition is complex, so it is hard to calculate the density of electrolyte.

b. The 1 M $Mg(Tf)_2$ in EC/PC (1/1 vol/vol) is mixed with PVDF-HFP with mass ratio of 80/20. The $MgAl_2O_4$ is added to polymer electrolyte with a 20 wt% weight of composite electrolyte. The density of this composite electrolyte is approxcimated as follows:

$$m_{solution} = \left(1.321\frac{g}{ml} * 500ml + 1.204\frac{g}{ml} * 500ml + 322.44\frac{g}{mol} * 1\,mol\right) = 1584.94\ g$$

$$m_{PVDF-HFP} = m_{solution} * \frac{20}{80} = 396.235\ g$$

$$m_{\mathrm{MgAl2O4}} = (m_{solution} + m_{PVDF-HFP}) * \frac{20}{80} = 495.29375\ g$$

$$\rho_{SSE} = \frac{m_{solution}+m_{PVDF-HFP}+m_{\mathrm{MgAl2O4}}}{V_{solution}+V_{PVDF-HFP}+V_{\mathrm{MgAl2O4}}} = \frac{1584.94\ g+495.29375\ g+495.29375\ g}{1000\ cm^{-3}+\frac{396.235\ g}{1.77\ g\ cm^{-3}}+\frac{495.29375\ g}{3.64\ g\ cm^{-3}}} = 1.821\ g\ cm^{-3})$$

Table S3. The parameters for an ideal cell with 100 wt % sulfur content and 100% S utilization. Porosity in cathode is 60 vol.%. Separator has 55 vol.% porosity.

Composites	Parameters
Carbon coated Al foil	0.0018 cm
Sulfur content	100%
Mg metal capacity excess	20%
Average operating voltage	1.77V
S utilization	100%
S areal loading (mg cm^{-2})	m_s
Electrolyte volume/S weight (μL/mg$_S$)	$\frac{E}{S}$
Celgard2500 thickness (μm)	25
Cathode tab, anode tab	Ni foil, 48 mm*4 mm*0.09 mm (160 mg/pcs)
Al laminate film	$13\text{cm} * 9\text{cm} * 0.0068\text{cm}$ [a]

(a. The area of Al laminate film (13 cm * 9 cm) is larger than the cross section of cell (12 cm * 8 cm) considering the cell sealing.)

Table S4. Mass (g) of each component of ideal Mg/S cell with height of 12 cm and width of 8 cm for gravimetric energy density simulation.

Components	**Mass (g)**
Carbon coated Al foil	$4.37 * 10^{-3} * 96$
Sulfur cathode	$m_s * 10^{-3} * 96$
Liquid electrolyte	$m_s * \frac{E}{S} * 10^{-3} * 1 * 96$
Celgard 2500	$0.0025 * 45\% * 0.946 * 96$
Mg anode	$\frac{1672 * m_s * 10^{-3} * 1.2 * 96}{2205}$
Al laminated film	$0.0068 * 1.75 * 2 * 13 * 9$
Cathode/anode tab (Ni tabs)	$0.16 * 2$
Total	$\left(0.183 + 0.096 * \frac{\mathrm{E}}{\mathrm{S}}\right) * m_s + 3.626$
Gravimetric energy density (Wh kg^{-1})	$\boldsymbol{\frac{1.77 * 1672 * m_s * 10^{-3} * 96}{\left(0.183 + 0.096 * \frac{E}{S}\right) * m_s + 3.626}}$

Table S5. Thickness (cm) of each component of ideal Mg/S cell for volumetric energy density simulation.

Components	Thickness (cm)
Carbon coated Al foil	0.0018
Sulfur cathode	$\frac{m_s * 10^{-3}}{2.07 * 40\%}$
Celgard 2500	0.0025
Mg anode	$\frac{1672 * m_s * 10^{-3} * 1.2}{2205 * 1.738}$
Al laminated film	0.0068*2
(Below values with electrolyte volume is less than pores volume of cathode and seperator)	
Liquid electrolyte outside pore	0
Cell thickness	$0.0179 + 1.732 * 10^{-3} * m_s$
Cell volumetric energy density (Wh L^{-1})	$\frac{1.77 * 1672 * m_s * 10^{-3} * 96}{(1.732 * 10^{-3} * m_s + 0.0179) * 96}$
(Below values with electrolyte volume is no less than pores volume of cathode and separator)	
Liquid electrolyte outside pore	$m_s * \frac{E}{S} * 10^{-3} - \frac{m_s * 10^{-3}}{2.07 * 40\%} * 60\% - 25 * 10^{-4} * 55\%$
Cell thickness	$\left(16.525 + 1.007 * m_s + m_s * \frac{E}{S}\right) * 10^{-3}$
Cell volumetric energy density (Wh L^{-1})	$\boldsymbol{\frac{1.77 * 1672 * m_s * 10^{-3} * 96}{\left(16.525 + 1.007 * m_s + m_s * \frac{E}{S}\right) * 10^{-3} * 96}}$

Table S6. The parameters for a realistic cell with 64 wt % sulfur content and 60.8% S utilization. The cathode has 60 vol.% porosity. Separator has 55 vol.% porosity.

Composites	**Parameters**
Carbon coated Al foil	0.0018 cm
Sulfur content	64%
Carbon nanotube content	16 wt%
Super-P content	10 wt%
PVDF content	10 wt%
Mg metal capacity excess	20%
Average operating voltage	1.2 V
S utilization	60.8%
S areal loading (mg cm-2)	m_s
Electrolyte volume/S weight (μL/mg$_S$)	$\frac{E}{S}$
Celgard2500 thickness (μm)	25
Cathode tab, anode tab	Ni foil, 48 mm*4 mm*0.09 mm (160 mg/pcs)
Al laminate film	$13\text{cm} * 9\text{cm} * 0.0068\text{cm}$

Table S7. Mass (g) of each component of realistic Mg/S cell with varied S loading and E/S ratio for gravimetric energy density simulation.

Components	**Mass (g)**
Carbon coated Al foil	$4.37 * 10^{-3} * 96$
Sulfur active material	$m_s * 10^{-3} * 96$
Carbon nanotube+Super-P+PVDF	$m_s * \frac{36}{64} * 10^{-3} * 96$
Liquid electrolyte	$m_s * \frac{E}{S} * 10^{-3} * 1 * 96$
Celgard 2500	$0.0025 * 45\% * 0.946 * 96$
Mg anode	$\frac{1019 * m_s * 10^{-3} * 1.2 * 96}{2205}$
Al laminated film	$0.0068 * 1.75 * 2 * 13 * 9$
Cathode/anode tab (Ni tabs)	$0.16 * 2$
Total	$\left(0.203 + 0.096 * \frac{E}{S}\right) * m_s + 3.626$
Gravimetric energy density (Wh kg^{-1})	$\boldsymbol{\frac{1.2 * 1019 * m_s * 10^{-3} * 96}{\left(0.203 + 0.096 * \frac{E}{S}\right) * m_s + 3.626}}$

Table S8. Thickness (cm) of each component of realistic Mg/S cell with varied S loading and E/S ratio for volumetric energy density simulation (Ignore the two tabs volume).

Components	**Thickness (cm)**
Carbon coated Al foil	0.0018
cathode	$\frac{\frac{m_s * 10^{-3}}{64\%} * (\frac{64\%}{2.07} + \frac{16\%}{2.1} + \frac{10\%}{1.9} + \frac{10\%}{1.78})}{1 - 60\%}$
Celgard 2500	0.0025
Mg anode	$\frac{1019 * m_s * 10^{-3} * 1.2}{2205 * 1.738}$
Al laminated film	$0.0068 * 2$
(Below values with electrolyte volume is less than pores volume of cathode and seperator)	
Liquid electrolyte outside pore	0
Cell thickness	$(17.9 + 3.264 * m_s) * 10^{-3}$
Cell volumetric energy density (Wh L^{-1})	$\frac{1.2 * 1019 * m_s * 10^{-3} * 96}{(17.9 + 3.264 * m_s) * 10^{-3} * 96}$
(Below values with electrolyte volume is no less than pores volume of cathode and separator)	
Liquid electrolyte outside pore	$m_s * \frac{E}{S} * 10^{-3} - 2.945 * 10^{-3} * m_s * 60\% - 25 * 10^{-4} * 55\%$
Cell thickness	$\left(16.525 + 1.497 * m_s + m_s * \frac{E}{S}\right) * 10^{-3}$
Cell volumetric energy density (Wh L^{-1})	$\boldsymbol{\frac{1.2 * 1019 * m_s * 10^{-3} * 96}{\left(16.525 + 1.497 * m_s + m_s * \frac{E}{S}\right) * 10^{-3} * 96}}$

Table S9. Mass (g) of each component of Mg/S cell for gravimetric energy density simulation with varied sulfur content and discharge capacity. (S loading is 6 mg cm^{-2}, E/S=3 μL mg^{-1}, and V_{dis}=1.77 V)

Components	Mass (g)
Carbon coated Al foil	$4.37 * 10^{-3} * 96$
Sulfur active material	$6 * 10^{-3} * 96$
Carbon nanotube+Super-P+PVDF	$6 * 10^{-3} * 96 * (1 - w_s)/w_s$
Liquid electrolyte	$6 * 3 * 10^{-3} * 1 * 96$
Celgard 2500	$0.0025 * 45\% * 0.946 * 96$
Mg anode	$\frac{C_{dis} * 6 * 10^{-3} * 1.2 * 96}{2205}$
Al laminated film	$0.0068 * 1.75 * 2 * 13 * 9$
Cathode/anode tab (Ni tabs)	$0.16 * 2$
Total	$0.576 * \frac{1 - w_s}{w_s} + 3.135 * 10^{-4} * C_{dis} + 5.93$
Gravimetric energy density (Wh kg^{-1})	$\boldsymbol{\frac{1.77 * C_{dis} * 6 * 10^{-3} * 96}{0.576 * \frac{1 - w_s}{w_s} + 3.135 * 10^{-4} * C_{dis} + 5.93}}$

Table S10. Thickness (cm) of Mg/S cell for volumetric energy density simulation with varied sulfur content and discharge capacity. (S loading is 6 mg cm^{-2}, and E/S=3 μL mg^{-1}, and V_{dis}=1.77 V)

Components	**Thickness (cm)**
Carbon coated Al foil collector	0.0018
Cathode	$\frac{\frac{6*10^{-3}}{w_s}(\frac{w_s}{2.07}+\frac{(90\%-w_s)*\frac{16}{26}}{2.1}+\frac{(90\%-w_s)*\frac{10}{26}}{1.9}+\frac{10\%}{1.78})}{1-60\%}$
Celgard 2500	0.0025
Mg anode	$\frac{C_{dis}*6*10^{-3}*1.2}{2205*1.738}$
Al laminated film	$0.0068*2$
(Below values with electrolyte volume is less than pores volume of cathode and seperator, which means $\boldsymbol{w_s<27}$%)	
Liquid electrolyte	0
Cell thickness	$\left(\frac{7.5315*10^{-3}}{w_s}+1.879*10^{-6}*C_{dis}+0.017714\right)$
Cell volumetric energy density (Wh kg^{-1})	$\boldsymbol{\frac{1.77*C_{dis}*6*10^{-3}*96}{\left(\frac{7.5315*10^{-3}}{w_s}+1.879*10^{-6}*C_{dis}+0.017714\right)*96}}$
(Below values with electrolyte volume is less than pores volume of cathode and seperator, which means $\boldsymbol{w_s>27}$%)	
Liquid electrolyte	$6*3*10^{-3}-t_{cathode}*60\%-t_{sep}*55\%$
Cell thickness	$\left(\frac{3.0126*10^{-3}}{w_s}+1.879*10^{-6}*C_{dis}+0.0334406\right)$
Volumetric energy density (Wh L^{-1})	$\boldsymbol{\frac{1.77*C_{dis}*6*10^{-3}*96}{(\frac{3.0126*10^{-3}}{w_s}+1.879*10^{-6}*C_{dis}+0.0344506)*96}}$

Table S11. Parameters of solid-state Mg/S battery for energy estimation.

Composites	**Parameters**
Carbon coated Al foil	0.0018 cm
Sulfur content	50 wt%
Super-P content	13.3 wt%
PVDF content	10 wt%
SSE content in cathode	26.7%
Thickness of each SSE (**μm**)	$varible$ (t)
Mg metal capacity excess	20%
Thickness of each Al laminated film (**μm**)	68
Cathode/anode tab (Ni tabs) (g)	0.16
Number of double-sided coated cathode	8
Number of SSE	16
Number of anode	16
Number of cathode current collector	8
Average operating voltage	1.2 V
S utilization	60.8%
S areal loading (mg cm^{-2})	$varible\ (m_s)$

Table S12. Mass (g) of each component of solid-state Mg/S cell with varied S loading and thickness of SSE for gravimetric energy density simulation.

Components	**Mass (g)**
Carbon coated Al foil	$4.37 * 10^{-3} * 96 * 8$
Sulfur active material	$m_s * 10^{-3} * 96 * 16$
PVDF[a]	$\frac{m_s}{50\%} * 10\% * 10^{-3} * 96 * 16$
Super-P[b]	$\frac{m_s}{50\%} * 13.3\% * 10^{-3} * 96 * 16$
Solid-state electrolyte	$\frac{m_s}{50\%} * 26.7\% * 10^{-3} * 96 * 16 + \mathrm{t} * 10^{-4} * 96 * 1.821 * 16$
Mg anode[c]	$\frac{1019 * m_s * 10^{-3} * 1.2 * 96}{2205} * 16$
Al laminated film	$0.0068 * 1.75 * 2 * 13 * 9$
Cathode/anode tab (Ni tabs)	$0.16 * 2$
Total mass[d]	$3.9238 * m_s + 0.2797 * t + 6.4608$
Gravimetric energy density (Wh kg^{-1})[e]	$\boldsymbol{\frac{1.2 * 1019 * m_s * 10^{-3} * 96 * 16}{3.9238 * m_s + 0.2797 * t + 6.4608}}$

(a. Sulfur content is 50wt% in cathode. b. PVDF content is 10wt% in cathode. Besides S and PVDF, the weight ratio of super-P and SSE is controded as 1:2 in cathode. c. The capacity ratio of Mg anode and S in cathode is 1.2. d. The number of double-sided coated cathode is 8, and the number of SSE and anode in a pouch cell are 16, respectively. e. The discharge capacity and the average discharge voltage are assumed as 1019 mAh g-1 and 1.2 V, same as pouch cell with liquid electrote.)

Table S13. Thickness (cm) of each component of solid-state Mg/S cell with varied S loading and thickness of SSE for volumetric energy density simulation (Ignore the two tabs volume).

Components	**Thickness (cm)**
Carbon coated Al foil	$0.0018 * 8$
Cathode	$\frac{\frac{m_s}{50\%} * 10^{-3} * (\frac{50\%}{2.07} + \frac{10\%}{1.78} + \frac{13.3\%}{1.9} + \frac{26.7\%}{1.821})}{1 - P} * 16$
Solid-state electrolyte	$\mathrm{t} * 10^{-4} * 16$
Mg anode	$\frac{1019 * m_s * 10^{-3} * 1.2}{2205 * 1.738} * 16$
Al laminated film	$0.0068 * 2$
Total	$2.4465 * 10^{-2} * m_s + 1.6 * 10^{-3} * t + 0.028$
Cell volumetric energy density (Wh L^{-1})	$\boldsymbol{\frac{1.2 * 1019 * m_s * 10^{-3} * 96 * 16}{(2.4465 * 10^{-2} * m_s + 1.6 * 10^{-3} * t + 0.028) * 96}}$

Table S14. Price of each material in Mg-S pouch cell.

Materials	Price
Mg metal	0.004 \$ g^{-1} (online price)
Sulfur	0.00022 \$ g^{-1} (online price)
Carbon nanotube	0.225 \$ g^{-1} (online price)
PVDF	0.01 \$ g^{-1} (online price)
Super-P	0.0068 \$ g^{-1} (online price)
Carbon coated Al foil	0.002 \$ cm^{-2} (MTI Corp.)
OMBB electrolyte	Variable \$ g^{-1}
Solid-state electrolyte (SSE)	Variable \$ g^{-1}
Celgard 2500	0.0001 \$ cm^{-2} (Alibaba good price)
Al laminated film	0.00002 \$ cm^{-2} (Alibaba good data)
Ni tab	0.6724 \$ pcs^{-1} (online price)
Ethylene carbonate (EC)	0.0907\$ g^{-1} (Sigma-Aldrich)
Propylene carbonate (PC)	141.1106 \$ L^{-1} (Sigma-Aldrich)
$Mg(Tf)_2$	5.92\$ g^{-1} (Sigma-Aldrich)
PVDF-HFP	0.9223 \$ g^{-1} (Sigma-Aldrich)
$MgAl_2O_4$	17.7935 \$ g^{-1} (Sigma-Aldrich)
anhydrous 1,2-dimethoxyethane (99.9%) (DME)	18 \$ L^{-1} (Chem impex website)
tris(hexafluoroisopropyl)borate (95%)	103.2 \$ g^{-1} (TCI)
anhydrous magnesium chloride (99.99%)	5 \$ g^{-1} (VWR website)
magnesium powder (99.8%)	0.2225 \$ g^{-1} (Alfa Aesar)

Table S15. Cost of each material in realistic Mg/S cell with liquid electrolyte. The realistic Mg/S cell has fixed average discharge voltage of 1.2V, S utilization of 60.8% (1019 mAh g^{-1}), E/S ratio of 3 μL mg^{-1}, and varied S loading m_s (mg cm^{-2}) and liquid electrolyte cost C_{elyt} ($ g^{-1}).

Composites	**Cost ($)**
Carbon coated Al foil	96 *0.002
Sulfur active material	$m_s * 10^{-3} * 96 * 0.00022$
Carbon nanotube	$m_s * \frac{16}{64} * 10^{-3} * 96 * 0.225$
Super-P	$m_s * \frac{10}{64} * 10^{-3} * 96 * 0.0068$
PVDF	$m_s * \frac{10}{64} * 10^{-3} * 96 * 0.01$
Liquid electrolyte	$m_s * 3 * 10^{-3} * 1 * 96 * C_{elyt}$
Celgard 2500	$96 * 0.0001$
Mg metal	$\frac{1019 * m_s * 10^{-3} * 1.2 * 96}{2205} * 0.004$
Al laminated film	$13 * 9 * 2 * 0.00002$
Cathode/anode tab (Ni tabs)	0.6724*2
Total	$0.005886 * m_s + 0.288 * m_s * C_{elyt} + 1.55058$
Cost per kWh	$\boldsymbol{\frac{0.005886 * m_s + 0.288 * m_s * C_{elyt} + 1.55058}{1.2 * 1019 * m_s * 10^{-3} * 96 * 10^{-6}}}$

Table S16. Cost of each material in Mg/S cell with solid-state electrolyte with thickness of solid-state electrolyte of 10 μm.

Composites	**Cost ($)**
Carbon coated Al foil	96 *8*0.002
Sulfur	$m_s * 10^{-3} * 96 * 16 * 0.00022$
PVDF	$\frac{m_s}{50\%} * 10\% * 10^{-3} * 96 * 16 * 0.01$
Super-P	$\frac{m_s}{50\%} * 13.3\% * 10^{-3} * 96 * 16 * 0.0068$
Solid-state electrolyte	$\left(\frac{m_s}{50\%} * 26.7\% * 10^{-3} * 96 + 10 * 10^{-4} * 96 * 1.821\right) * 16 * C_{SSE}$
Mg anode	$\frac{1019 * m_s * 10^{-3} * 1.2 * 96}{2205} * 16 * 0.004$
Al laminated film	$13 * 9 * 2 * 0.00002$
Cathode/anode tab (Ni tabs)	0.6724*2
Total cost	$(0.8202 * m_s + 2.797) * C_{SSE} + 6.18822 * 10^{-3} * m_s + 2.915767$
Cost per kWh	$\boldsymbol{\frac{(0.8202 * m_s + 2.797) * C_{SSE} + 6.18822 * 10^{-3} * m_s + 2.915767}{1019 * 1.2 * m_s * 10^{-3} * 96 * 10^{-6} * 16}}$

Price of 0.5 M organic magnesium borated-based electrolyte (OMBB) calculation

OMBB electrolytes were synthesized by reaction of $B(HFP)_3$, Mg powders and $MgCl_2$ in DME solvent. The volume of electrolytes is set as 1 L. The concentration of $B(HFP)_3$ is 0.5 M. The ratio of $B(HFP)_3$: $MgCl_2$ is 2:1, and Mg powder is added in excess which is filtered finally. Therefore, the mole number of $B(HFP)_3$ and $MgCl_2$ are 0.5 and 0.25, respectively. Because the equilibrium species in the electrolyte is $[Mg_4Cl_6(DME)_6][B(HFP)_4]_2$, the mole ratio of Mg and B is 4:2, thus the reacted Mg powder is estimated to be 0.75 mole in this price calculation.

The price of the 0.5 M organic magnesium borated-based electrolyte (OMBB) is

$$\boldsymbol{Price_{OMBB}} = \frac{\boldsymbol{cost_{\mathrm{B(HFP)3}}} + \boldsymbol{cost_{\mathrm{MgCl2}}} + \boldsymbol{cost_{Mg\ powder}} + \boldsymbol{cost_{DME}}}{\boldsymbol{mass_{\mathrm{B(HFP)3}}} + \boldsymbol{mass_{\mathrm{MgCl2}}} + \boldsymbol{mass_{Mg\ powder}} + \boldsymbol{cost_{DME}}}$$

$$= \frac{\mathbf{0.5}\boldsymbol{mol} * \mathbf{511.9}\,\frac{\boldsymbol{g}}{\boldsymbol{mol}} * \mathbf{103.2}\,\frac{\$}{\boldsymbol{g}} + \mathbf{0.25}\boldsymbol{mol} * \mathbf{95.21}\,\frac{\boldsymbol{g}}{\boldsymbol{mol}} * \mathbf{5}\frac{\$}{\boldsymbol{g}} + \mathbf{0.75}\boldsymbol{mol} * \mathbf{24.3}\frac{\boldsymbol{g}}{\boldsymbol{mol}} * \mathbf{0.2225}\,\frac{\$}{\boldsymbol{g}} + \mathbf{18}\frac{\$}{\boldsymbol{L}} * \mathbf{1}\boldsymbol{L}}{\mathbf{0.5}\boldsymbol{mol} * \mathbf{511.9}\,\frac{\boldsymbol{g}}{\boldsymbol{mol}} + \mathbf{0.25}\boldsymbol{mol} * \mathbf{95.21}\,\frac{\boldsymbol{g}}{\boldsymbol{mol}} + \mathbf{0.75}\boldsymbol{mol} * \mathbf{24.3}\frac{\boldsymbol{g}}{\boldsymbol{mol}} + \mathbf{0.867}\frac{\boldsymbol{g}}{\boldsymbol{cm^3}} * \mathbf{1000}\,\boldsymbol{cm^3}}$$

$$= \mathbf{23}\ \$\ \boldsymbol{g^{-1}}$$

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