

Enhancing the cycling stability of Mg-SeS₂ batteries with an artificial electrode skin

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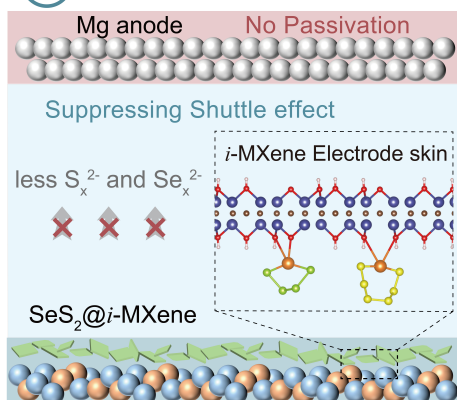
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😊 Enhanced Cycling Stability



The authors constructed an artificial electrode skin using *i*-MXene (Mo_{1.33}C) nanosheets for long-life Mg-SeS₂ batteries. The hydroxyl groups on the surface of *i*-MXene exhibit strong chemical adsorption with the intermediate products during the discharge process, effectively confining S_x²⁻/Se_x²⁻ within the cathode.

Enhancing the cycling stability of Mg-SeS₂ batteries with an artificial electrode skin

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ABSTRACT: Magnesium-sulfur (Mg-S) batteries typically exhibit high discharge capacity but suffer from poor cycling performance due to the shuttle effect of polysulfides. In this study, we develop an artificial electrode skin on the SeS₂ cathode in a Mg-SeS₂ battery to effectively suppress the shuttle of polysulfides and polyselenides. A range of electrochemical and spectroscopic characterizations are conducted to investigate the confinement effect of the *i*-MXene-based electrode skin on dissolved sulfur- and selenium-based species. Theoretical simulations indicate that surface hydroxyl groups and other functional moieties of *i*-MXene can effectively confine active species to the cathode side. As a result, the Mg-SeS₂ battery with the cathode skin layer demonstrates a high discharge capacity of 750 mAh g⁻¹ at a current density of 0.1 A g⁻¹, with excellent cycling stability. The battery maintains 76% of its capacity after 100 cycles at 0.5 A g⁻¹ and 62% after 300 cycles at 2 A g⁻¹, exceeding or matching the performance of most previously reported Mg-S batteries. This work demonstrates a viable strategy to boost the electrochemical performance of Mg-ion batteries.

KEYWORDS: Mg-SeS₂ batteries, Mo_{1.33}C, artificial electrode skin, shuttle effect, cycling stability

1 Introduction

Rechargeable magnesium-ion batteries (RMBs) have garnered significant attention due to the high abundance of magnesium (Mg) resources (~2% mass content in the Earth's crust) and the high volumetric capacity of Mg (3833 mAh cm⁻³) [1-3]. However, the development of intercalation-type RMB cathodes has been hindered by the strong electrostatic interactions between Mg²⁺ ions and the host anion lattice, resulting in a low specific capacity (usually < 200 mAh g⁻¹) [4, 5]. In contrast, conversion-type cathodes (such as sulfur-based materials) offer much higher theoretical capacities compared to traditional intercalation-type cathodes (1625 mAh g⁻¹ for S vs. 128 mAh g⁻¹ for Mo₆S₈) [6, 7]. As a result, magnesium-sulfur (Mg-S) batteries have emerged as a promising option for next-generation battery technologies.

Yet, Mg-S batteries face significant challenges, including the low utilization of polysulfide intermediates, primarily due to the polysulfide dissolution and the "shuttle effect" driven by the concentration gradient [8]. Several approaches have been proposed to mitigate this issue. One of the most

commonly used strategies is loading sulfur onto porous carbon materials to suppress the shuttle effect in Mg-S batteries. For example, Zhao-Karger et al. reported an ordered mesoporous carbon/sulfur (S/CMK-3) cathode for Mg-S batteries. Thanks to its large pore volume and interconnected pore structure, CMK-3 provides a confined space and conductive framework for the electrochemical reactions of sulfur. As a result, the Mg-S/CMK-3 batteries maintained a reversible discharge capacity of approximately 200 mAh g⁻¹ after 100 cycles at a current density of 0.167 A g⁻¹. Moreover, incorporating sulfur into cathode host materials via covalent bonding has been reported to effectively suppress polysulfide dissolution in the electrolytes [9, 10]. Mai and An's group demonstrated that hollow nanospheres of vanadium nitride acted as an effective sulfur host for high-performance Mg-S batteries [11]. The vanadium nitride provides a strong chemical anchoring effect for polysulfides, thereby facilitating the reaction kinetics of polysulfide conversion and suppressing the shuttle effect. The assembled battery exhibited good cycling stability, with 78% capacity retention after 100 cycles at a current density of 0.5 A g⁻¹. In addition, separator

engineering, such as modifying the separator with graphene, has also been used to capture dissolved polysulfides and suppress their diffusion to the anode side [8, 12]. Despite these pioneering achievements, developing effective strategies to suppress the shuttle effect in Mg-S batteries and further understanding the underlying mechanisms remain of significant interest and pose challenges for the scientific community.

In this study, we used a Ketjen black (KB)/SeS₂ composite as a superior cathode material for magnesium-ion batteries. The SeS₂ electrode leveraged the complementary properties of sulfur (high specific capacity) and selenium (high electronic conductivity), delivering a high discharge capacity of 750 mAh g⁻¹ at a current density of 0.1 A g⁻¹. However, the shuttling of polysulfides and polyselenides to the anode side during charge/discharge processes resulted in active material loss and anode passivation, leading to rapid capacity decay. Therefore, we fabricated an artificial electrode skin on the cathode surface using an *i*-MXene (Mo_{1.33}C) layer to prevent dissolved polysulfides and polyselenides from passing through the separator to the anode surface. Spectroscopic analysis, electrochemical testing, and theoretical simulations revealed that the hydroxyl groups on the *i*-MXene surface serve as the primary functional groups that effectively confine the intermediate products (polysulfides and polyselenides) on the cathode side. As a result, the assembled Mg-SeS₂ battery with the cathode skin layer demonstrated excellent cycling stability, retaining 76% of its capacity after 100 cycles at 0.5 A g⁻¹ and 62% of its capacity after 300 cycles at 2 A g⁻¹, providing new insights into the rational design of long-life batteries.

2 Results and discussion

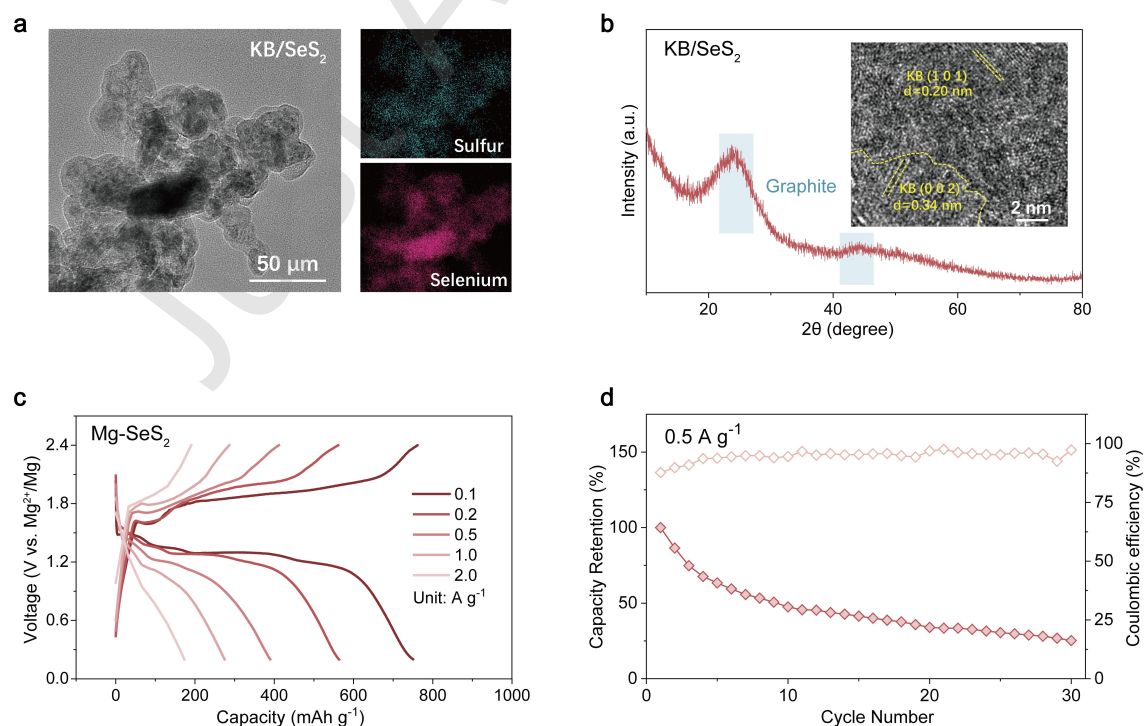


Figure 1. (a) TEM images for KB/SeS₂ and corresponding element mapping images. (b) XRD pattern and high-resolution TEM image of KB/SeS₂. (c) The galvanostatic charge/discharge curves of the Mg-SeS₂ battery from 0.1 to 2 A g⁻¹. (d) Cyclic stability of the battery at the current density of 0.5 A g⁻¹.

A KB/SeS₂ composite was fabricated as the cathode material via a melting method (Experimental Section in Supporting Information). The transmission electron microscopy (TEM) and corresponding element mapping images (Fig. 1(a)) confirm that the molten S and Se were uniformly coated on the surface of KB. N₂ adsorption-desorption isotherms of KB and the KB/SeS₂ materials suggest that the micro/mesopores of KB were filled with SeS₂ (Fig. S1 in the ESM). In addition to the diffraction peaks [(002) and (101) planes of graphite (JCPDF No. 75-1621)] for KB, we did not observe other diffraction signals (Fig. 1(b) and Fig. S2 in the ESM) in the XRD pattern of the KB/SeS₂ composite, indicating the amorphous nature of S and Se components. This is in good agreement with the high-resolution TEM image (inset in Fig. 1(b)). X-ray photoelectron spectroscopy (XPS) S 2p and Se 3p core-level spectra of the samples were collected (Fig. S3 in the ESM), which can be fitted into two components, i.e., S⁰ (163.9 eV, and 165.1 eV), and Se⁰ (162.2 eV, and 168.9 eV) [13]. The thermogravimetry (TG) analysis in Fig. S4 in the ESM indicates the weight percentage of SeS₂ in the composite is about 41.8%.

We assembled a Mg-SeS₂ battery using the KB/SeS₂ composite as the cathode, a piece of Mg foil as the anode, and 0.5 M Mg(TFSI)₂-diethyleneglycoldimethylether (DEGDME) solution as the electrolyte, respectively. Fig. 1(c) presents the charge/discharge profiles of the KB/SeS₂ battery. The KB/SeS₂ composite demonstrates a high specific capacity of 750 mAh g⁻¹ at a current density of 0.1 A g⁻¹. At a higher current density of 2 A g⁻¹, the KB/SeS₂ composite still delivers a discharge capacity of 173 mAh g⁻¹. However, the Mg-SeS₂ battery exhibits poor cycling stability, with 25% capacity retention after 30 cycles at a current density of 0.5 A g⁻¹ (Fig. 1(d)).

To investigate the underlying causes of battery failure, we conducted spectroscopic analysis to track the evolution of sulfur and selenium species during the discharge process (the selected test states are shown in Fig. 2(a)). The batteries at different discharge states were disassembled, and the electrolytes were extracted by immersing the separators in the corresponding solvent to conduct ex situ ultraviolet-visible spectroscopy (UV-vis) tests (Fig. 2(b)). At 1.5 V, only signals for elemental sulfur (S_8) and selenium (Se_8) were detected, consistent with the results reported by Zhao-Karger [10]. As discharge progressed, the characteristic peak for S_8 and Se_8 nearly disappeared, being replaced by peaks corresponding to polysulfides (S_x^{2-}) at 247 and 356 nm, and polyselenides (Se_x^{2-}) at 276, 312, and 328 nm [14, 15].

Ex-situ Raman spectroscopy was further employed to investigate the evolution of the S_x^{2-} species (Fig. 2(c)). Initially, the electrolyte contained only S_8 , consistent with the UV-vis results. Upon discharge to 1.3 V vs. Mg^{2+}/Mg , the peak

corresponding to S_6^{2-} appeared. Further discharge to 1.0 V vs. Mg^{2+}/Mg led to the complete disappearance of the S_6^{2-} signal, with only the S_4^{2-} signal remaining, indicating that S_6^{2-} had been reduced to S_4^{2-} [14]. It is worth noting that the peaks for Se_x^{2-} (at around 328 cm^{-1}) were obscured by the electrolyte peak, making it difficult to observe the Se_x^{2-} evolution during discharge via Raman tests [16]. The above spectroscopic results suggest that the S_x^{2-} and Se_x^{2-} species were dissolved in the electrolyte during the discharge of the Mg- SeS_2 battery. The dissolution of these active materials in the electrolyte would, therefore, lead to a decrease in capacity. The dissolution of these active materials in the electrolyte would, therefore, lead to a decrease in capacity. No distinct Raman signal at 375 cm^{-1} assigned to S-Se bonds were captured in our ex-situ measurements, implying that mixed S-Se chained intermediates are not substantially formed under the present operating conditions.

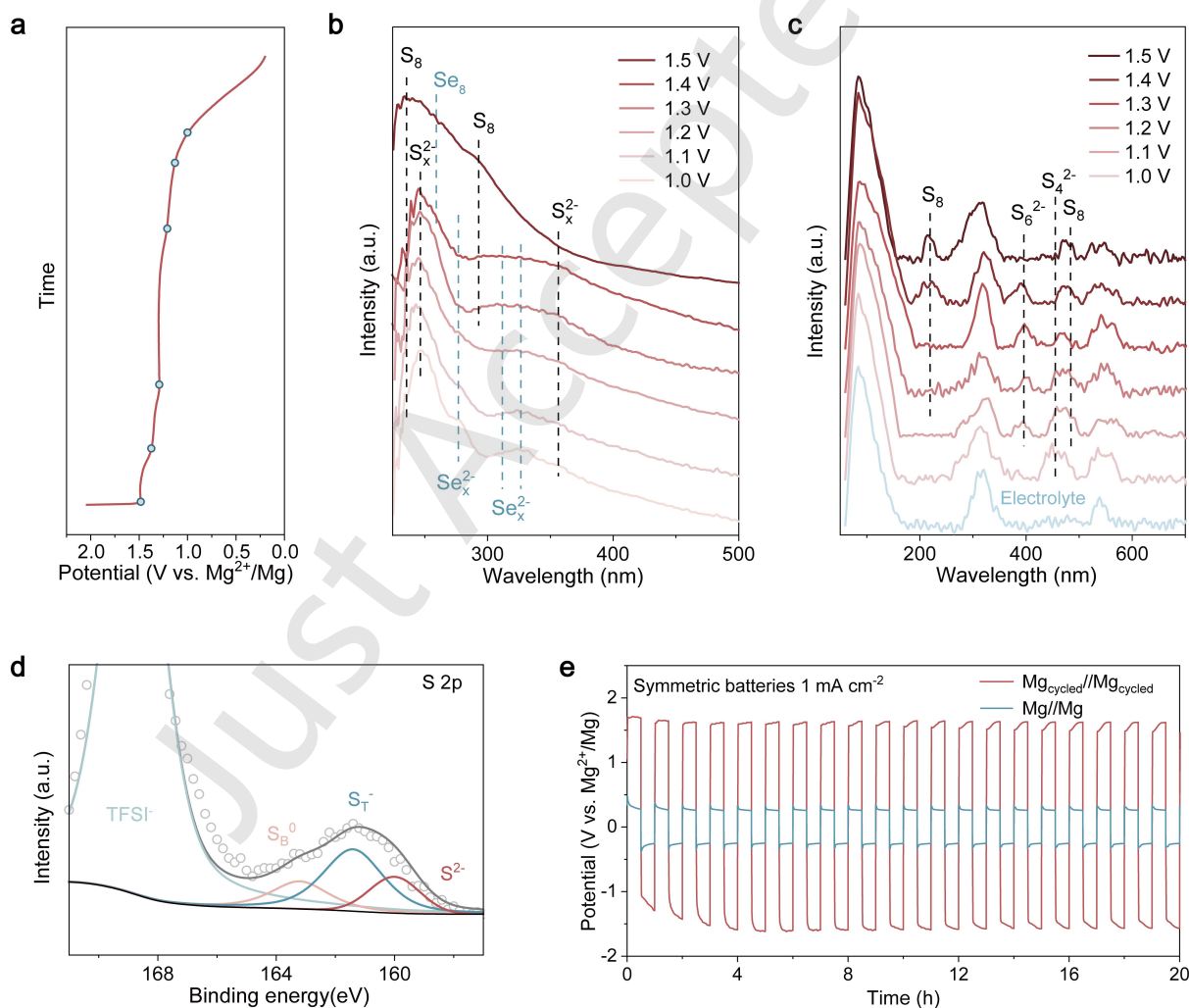


Figure 2. (a) The discharge curve of Mg- SeS_2 batteries at the current density of 0.1 A g^{-1} . (b) Ex-situ UV-vis spectra and (c) Raman spectra of electrolyte at different discharging states. (d) XPS S 2p spectra of the cycled Mg foil in Mg- SeS_2 batteries. (e) Cycling tests of the symmetric cells using the fresh Mg foil and cycled Mg foil in Mg- SeS_2 batteries, respectively.

The passivation of the anode can also cause capacity degradation of Mg- SeS_2 batteries [17]. To investigate this, XPS measurements were performed to characterize the surface chemical composition of the Mg anode after cycling (denoted as Mg_{cycled}). The XPS S 2p spectra of Mg_{cycled} revealed peaks corresponding to

Bis(trifluoromethanesulfonyl)imide (TFSI⁻) at 168.8 eV [18], terminal sulfur (S_T^{-1}) at 161.4 eV, bridging sulfur (S_B^0) at 163.3 eV, and sulfide (S^{2-}) at 160 eV (Fig. 2(d)) [19]. The presence of S_T^{-1} , S_B^0 , and S^{2-} signals indicate the formation of insoluble sulfide/polysulfide species on the Mg anode. Additionally, selenium signals were detected in the XPS Se 3d

spectrum (Fig. S5 in the ESM). These results suggest that the soluble S_x^{2-}/Se_x^{2-} species migrated through the separator to the anode, where they eventually form an insulating Se/S-based layer on the Mg surface. This insulating layer passivates the Mg anode, leading to a significant increase in electrochemical polarization (Fig. 2(e)). Therefore, suppressing the shuttle effect of the dissolved S_x^{2-}/Se_x^{2-} species presents a promising strategy to enhance the cycling stability of Mg-S batteries [20].

MXenes, with their rich polar surface functional groups (such as -OH, -F, and -Cl), may exhibit great potential for capturing polysulfides [21]. By using the heavy rare-earth elements (such as Y) in the synthesis of MAX precursor, $(Mo_{2/3}Y_{1/3})_2AlC$ *i*-MAX phase can be obtained with Y ordered occupation [22]. By conventional aqueous etching and delamination, Y and Al will be etched and the high density of topological ordered vacancies will appear on $Mo_{1.33}C$ *i*-MXene, which is expected to enhance the active surface area and

facilitate Mg^{2+} diffusion (Fig. 3(a)). Therefore, we fabricated an *i*-MXene ($Mo_{1.33}C$) electrode skin to prevent the migration of dissolved polysulfides/polyselenides to the anode.

$Mo_{1.33}C$ *i*-MXene, derived from $(Mo_{2/3}Y_{1/3})_2AlC$ *i*-MAX phase, is presented in Fig. S6 in the ESM. The (002) peak at a lower angle indicates a wide lattice spacing of 14.5 Å following delamination. The XPS Mo 3d spectrum of $Mo_{1.33}C$ *i*-MXene exhibited peaks corresponding to Mo^{6+} , Mo^{5+} , and Mo-C, consistent with previous reports (Fig. S7 in the ESM) [22]. XPS spectra were also collected to identify the functional groups on the surface of the *i*-MXene (Fig. S8 in the ESM). The unique peak in XPS O 1s spectrum corresponds to the Mo-O-H bond, confirming the high degree of hydroxylation on the *i*-MXene surface [23]. The XPS F 1s and Cl 2p spectra provide evidence for the incorporation of -F and -Cl functional groups [24, 25]. Additionally, SEM and TEM images (Fig. 3(b) and Fig. S9 in the ESM) indicate the successful fabrication of few-layer *i*-MXene.

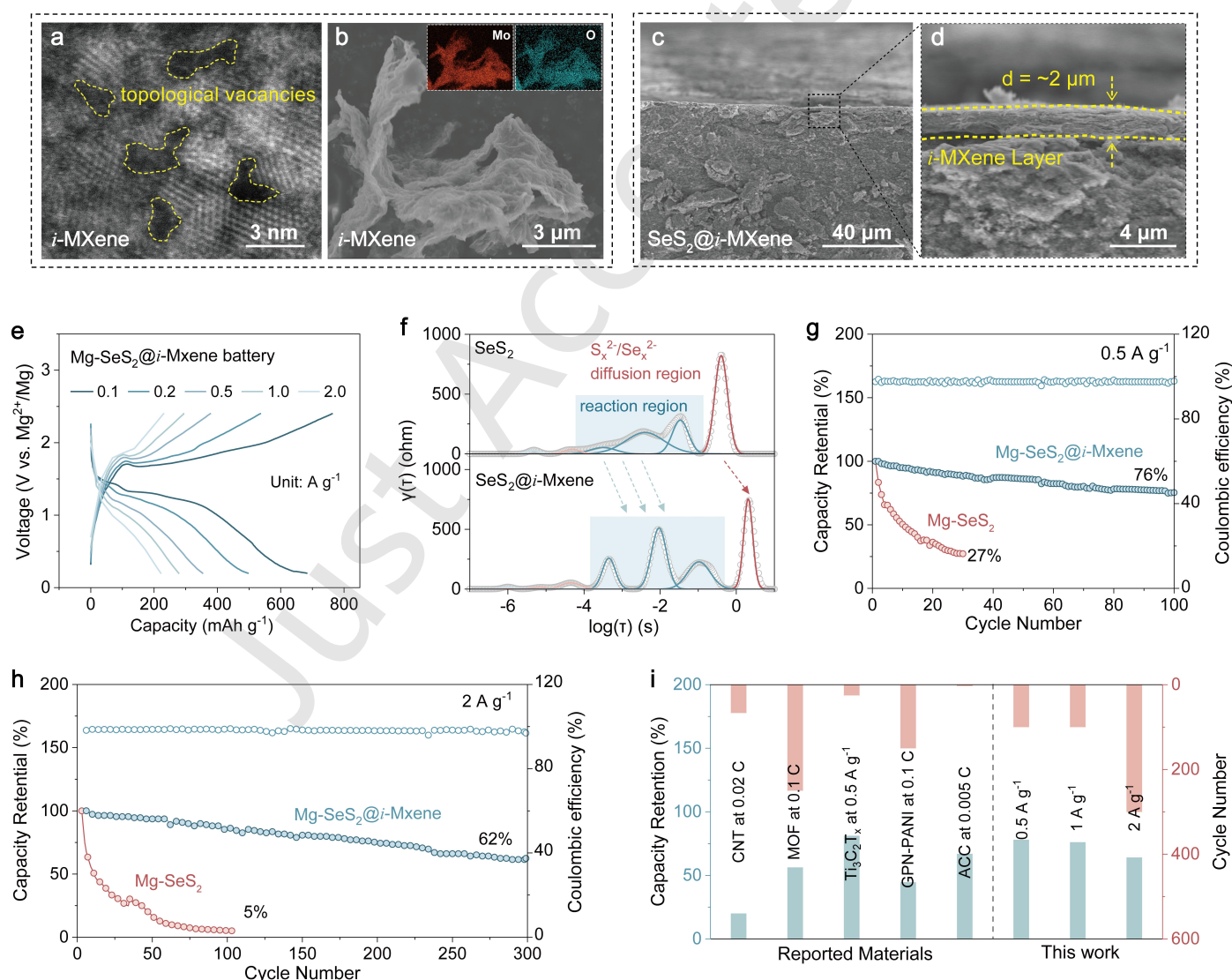


Figure 3. (a) High-resolution transmission electron microscope image of *i*-MXene. (b) SEM image and corresponding element mapping images for *i*-MXene. (c-d) SEM images of the $SeS_2@i$ -MXene electrode cross-section. (e) The galvanostatic charge/discharge curves of $Mg-SeS_2@i$ -MXene batteries from 0.1 to 2 $A\ g^{-1}$. (f) The distribution of relaxation times (DRT) analysis of $Mg-SeS_2$ batteries and $Mg-SeS_2@i$ -MXene batteries. (g) Cycling stability of $Mg-SeS_2$ batteries and $Mg-SeS_2@i$ -MXene batteries at a current density of 0.5 $A\ g^{-1}$, and (h) 2 $A\ g^{-1}$. (i) A comparison of the cycling stability of our work with that of other reported Mg-S batteries using different functional materials.

We then fabricated the *i*-MXene electrode skin on the SeS₂ electrode using a drop-casting method (Experimental Section in Supporting Information). The as-prepared electrode was denoted as SeS₂@*i*-MXene. The thickness of the *i*-MXene layer is about ~2 μm with a mass loading of 1 mg cm⁻² (Fig. 3(c) and 3(d)). It is worth noting that this cathode-surface artificial skin design is distinct from conventional separator modification strategies. The *i*-MXene skin achieves intimate conformal contact with cathode particles and deforms synchronously with active materials during cycling. Such structural superiority effectively avoids mechanical mismatch and coating delamination, whereas separator coatings merely offer indirect physical isolation. The assembled Mg-SeS₂@*i*-MXene battery exhibits a specific capacity of 683 mAh g⁻¹ at the current density of 0.1 A g⁻¹ with a energy efficiency of 47.1% (Fig. 3(e)), which is similar to that of the battery without the *i*-MXene layer. It is noted that the *i*-MXene layer provide negligible capacity to the overall capacity of the electrode (Fig. S10 in the ESM). The electrochemical impedance spectroscopy (EIS) spectra suggest that the Mg-SeS₂@*i*-MXene battery exhibits a slightly higher charge transfer resistance compared to the Mg-SeS₂ battery (Fig. S11 in the ESM), indicating that the *i*-MXene skin helps mitigate the charge transfer at the electrode surface [26]. Consistent with Lewis acid-base interactions, the abundant polar surface functional groups (-OH, -F, -Cl) on *i*-MXene enable strong anchoring of polysulfide/polyselenide species while introducing interfacial barriers for Mg²⁺ migration. Upon incorporation of the *i*-MXene layer, the relaxation time within the diffusion region extends from 10^{-0.38} to 10^{0.32} s, signifying elevated diffusion impedance of mobile ions. This phenomenon is

further corroborated by EIS and CV measurements, which demonstrate increased charge-transfer resistance and aggravated polarization for Mg-SeS₂@*i*-MXene batteries (Fig. S12 in the ESM). Nevertheless, despite the polarization penalty arising from Mg²⁺ interfacial obstruction, the protected cathode achieves improved rate performance. The *i*-MXene skin effectively suppresses the shuttle of soluble intermediates and mitigates active material dissolution. These favorable effects outweigh the kinetic drawbacks stemming from hindered Mg²⁺ transport, yielding enhanced capacity retention under various current densities (Fig. S13 in the ESM). Importantly, the cycling stability of the Mg-SeS₂@*i*-MXene battery was significantly improved, achieving 76% capacity retention after 100 cycles at a current density of 0.5 A g⁻¹ (Fig. 3(g)). When the current density is increased to 1 and 2 A g⁻¹, the capacity retention remains 78% (100 cycles) and 62% (300 cycles), respectively, which is notably better than that of the Mg-SeS₂ battery (Fig. 3(h) and Fig. S14 in the ESM). Moreover, the average Coulombic efficiency of the Mg-SeS₂@*i*-MXene battery consistently exceeds 99%. These results outperform or are comparable to those reported for Mg-S batteries (Fig. 3(i)) [12, 28-31]. Further electrochemical tests quantitatively verify the prominent cycling stability and anti-shuttle capability of the *i*-MXene-modified cathode. The rate-recovery test demonstrates that the capacity retention rises from 57% for the bare KB/SeS₂ cathode to 83% after introducing the *i*-MXene skin (Fig. S15 in the ESM). Moreover, the self-discharge measurement confirms that the modified cell still maintains a satisfactory Coulombic efficiency of 75% after 12 h of resting (Fig. S16 in the ESM), further proving the effective inhibition of soluble intermediate leakage and shuttle-induced side reactions.

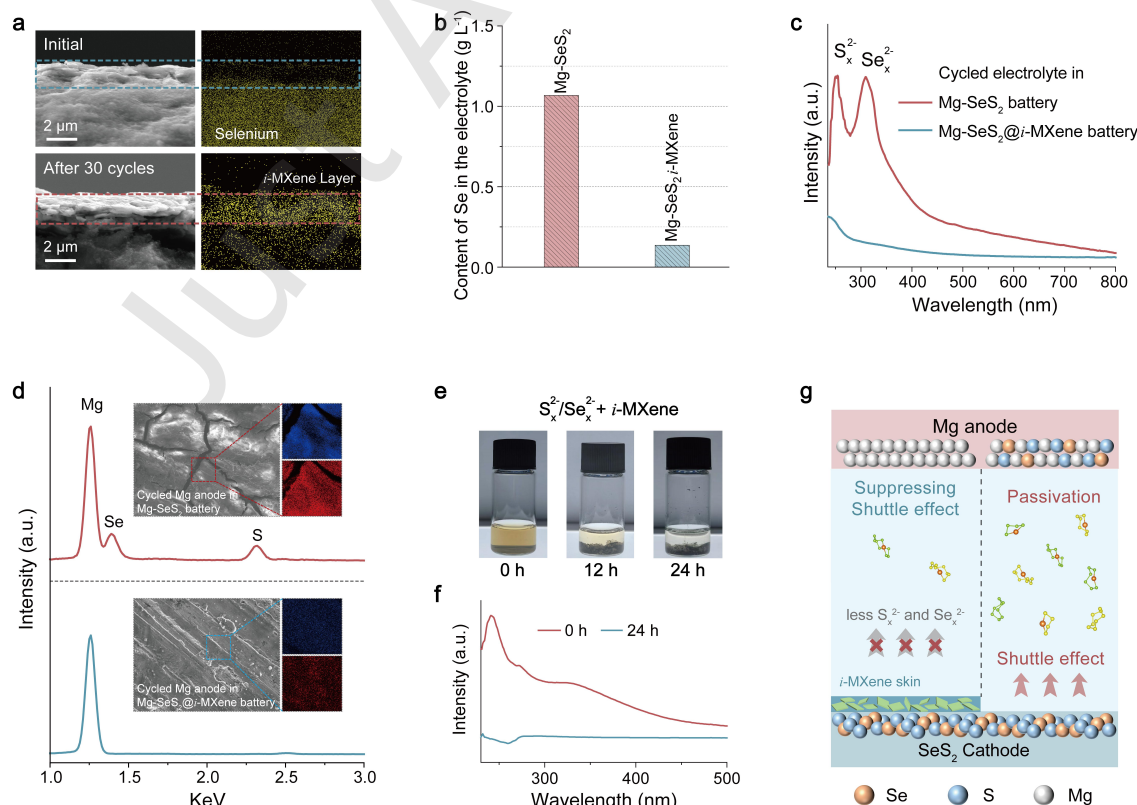


Figure 4. (a) SEM and corresponding element mapping images for the SeS₂@*i*-MXene electrode before and after cycling. (b) ICP-OES results, and (c) UV-vis spectra for the cycled electrolytes in Mg-SeS₂ and Mg-SeS₂@*i*-MXene batteries. (d) EDX spectra of the cycled Mg anode in the Mg-SeS₂ and Mg-SeS₂@*i*-MXene

batteries, inset shows the SEM images and corresponding element mapping images. (e) The digital photos of the solution containing dissolved S_x^{2-}/Se_x^{2-} species and *i*-MXene at 0 h, 12 h, and 24 h, and (f) the UV-vis spectra for the solutions. (g) Schematic illustration of MXene skin suppressing the shuttle effect.

To investigate the protective effect of the *i*-MXene skin, we collected cross-sectional elemental mapping images of the $SeS_2@i$ -MXene electrode before and after cycling for 30 cycles, as shown in Fig. 4(a) and Fig. S17 in the ESM. Before cycling, no Se signal is detected in the electrode surface layer. Interestingly, after cycling, the Se signal extends to the surface layer, and its distribution in the surface layer is stronger than that in the electrode bulk, indicating that Se-based species were trapped at the electrode surface during the charge/discharge process. This suggests strong chemical adsorption of polyselenides by the *i*-MXene layers. Note that the energy-dispersive X-ray (EDX) spectrum cannot distinguish between Mo and S due to their similar energy levels, which complicates the demonstration of polysulfide adsorption on *i*-MXene. However, the relative intensity evolution of S/Mo composite mapping still provides valid qualitative information. For the pristine electrode, the outer *i*-MXene skin mainly shows Mo signals, whereas sulfur signals from SeS_2 dominate the cathode bulk. After 30 cycles, the bulk cathode exhibits weakened sulfur signals, indicating severe dissolution of SeS_2 species in the electrode without the protective skin. Meanwhile, the *i*-MXene surface layer displays enhanced signal intensity, originating from the superposition of intrinsic Mo signals and sulfur signals from trapped polysulfide intermediates. (Fig. S17 in the ESM). To eliminate the spectral ambiguity induced by EDX peak overlap and clarify the interfacial trapping behavior of sulfur-containing intermediates, ex situ high-resolution S 2p XPS measurements were conducted on the *i*-MXene skin layer disassembled from electrodes after 30 cycles. Distinct characteristic polysulfide signals were clearly detected on the cycled *i*-MXene surface, directly verifying that the artificial skin can effectively immobilize soluble sulfur intermediates during cycling (Fig. S18 in the ESM). Inductively coupled plasma optical emission spectroscopy (ICP-OES) measurements were conducted to test the Se content in the electrolyte after cycling both Mg- SeS_2 and Mg- $SeS_2@i$ -MXene batteries. The soluble Se content in the electrolyte decreased significantly after coating the *i*-MXene skin on the SeS_2 electrode (Fig. 4(b)). Note that, since the

TFSI⁻-based electrolyte contains sulfur, ICP analysis faced difficulties in measuring the amount of polysulfides in solution. The ultraviolet-visible (UV-vis) spectra in Fig. 4(c) show that significant amounts of S_x^{2-} and Se_x^{2-} are dissolved in the electrolyte of the Mg- SeS_2 battery, leading to rapid capacity decay. In contrast, the electrolyte of the Mg- $SeS_2@i$ -MXene batteries contains almost no S_x^{2-} and Se_x^{2-} , indicating that the *i*-MXene layer effectively confines the dissolved polysulfides and polyselenides on the cathode side, thereby suppressing the shuttle effect. SEM and the corresponding EDX results show significant S and Se signals on the cycled anode surface of the Mg- SeS_2 battery (Fig. 4(d)). In contrast, the anode of the Mg- $SeS_2@i$ -MXene battery after cycling exhibits negligible S and Se signals, further indicating that the *i*-MXene layer effectively suppresses the shuttle of polysulfides and polyselenides, thereby preventing anode passivation from polysulfide and polyselenide shuttling (Fig. S19 in the ESM). We further conducted a visual adsorption and spectroscopic experiment using a solution containing dissolved polysulfides and polyselenides, prepared via electrochemical methods (details can be found in the Experimental Section of the Supporting Information). 10 mg of *i*-MXene was added to the solution and allowed to stand for 24 hours, as shown in the inset of Fig. 4(e). The transparency of the solution gradually increased with time, indicating that *i*-MXene effectively adsorbed the S_x^{2-} and Se_x^{2-} species. UV-vis spectroscopy further confirmed this observation, with the absorption peaks corresponding to S_x^{2-} and Se_x^{2-} disappearing after 24 hours (Fig. 4(f)). To rule out the possibility that the spectral changes originate from redox reactions, material decomposition or precipitation instead of adsorption, we performed XPS characterization on the solid *i*-MXene after the static adsorption test. Distinct characteristic signals of soluble polysulfide/polyselenide species are clearly detected on the surface of post-adsorption *i*-MXene, directly verifying that the dissolved sulfur/selenium intermediates are immobilized onto the *i*-MXene surface (Fig. S20 in the ESM). The above results all confirm the confinement effect of MXene skin on polysulfides and polyselenides (Fig. 4(g)).

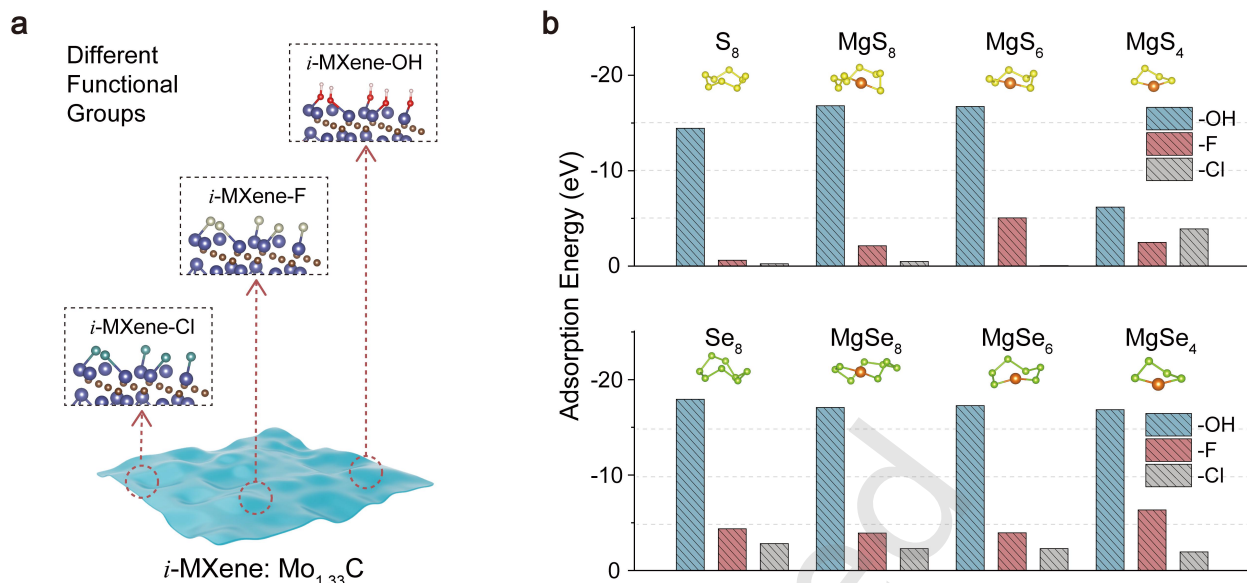


Figure 5. (a) Schematic illustration of different functional groups on the surface of i -MXene. The adsorption energies of (b) S-related species and Se-related species on the i -MXene with different functional groups.

Density functional theory (DFT) calculations were conducted to study the interaction mechanism between the i -MXene skin and the S_x^{2-} and Se_x^{2-} species. During the etching and post-treatment processes, various functional groups (such as -OH, -F, and -Cl) are incorporated onto the surface of $\text{Mo}_{1.33}\text{C}$, significantly influencing its physicochemical properties (Fig. 5(a) and Fig. S21 in the ESM) [32]. It should be noted that the DFT models employ ideally fully monofunctionalized i -MXene surfaces (-OH, -F, -Cl), representing an extreme high-coverage limit. These calculations are intended for comparative analysis of group-dependent interaction strength, instead of providing quantitative absolute adsorption energies for the experimentally obtained mixed-termination i -MXene. Real $\text{Mo}_{1.33}\text{C}$ i -MXene possesses randomly distributed mixed-functional groups with lower surface coverage. The adsorption energies of S- and Se-related species on the i -MXene with different functional groups are shown in Fig. 5(b), and S16 in the ESM. All these species exhibit strong interactions with the functionalized i -MXene materials, particularly for the -OH functionalized i -MXene [33]. These results explain why the i -MXene skin can trap dissolved polysulfides and polyselenides on the cathode side, thereby suppressing the shuttle effect [34]. The i -MXene layer prevents active material loss and anode passivation during the charge/discharge process, leading to enhanced cycling stability for the Mg battery.

3 Conclusions

In summary, we constructed an artificial electrode skin using i -MXene ($\text{Mo}_{1.33}\text{C}$) nanosheets for long-life Mg-Se S_2 batteries. The dissolution and shuttle behavior of polysulfides and polyselenides was suppressed effectively. Therefore, the assembled Mg-Se S_2 @ i -MXene battery demonstrates high discharge capacity of 683 mAh g^{-1} at the current density of 0.1 A g^{-1} . In addition, it delivers a 76% capacity retention at the current density of 0.5 A g^{-1} over 100 cycles and a 62% capacity retention at the current density of

2 A g^{-1} over 300 cycles, providing new insights into the rational design of long-life Mg-S batteries. Theoretical calculations demonstrate that the functional groups including hydroxyl groups on the surface of i -MXene exhibit strong chemical adsorption with the intermediate products during the discharge process, effectively confining S_x^{2-} / Se_x^{2-} within the cathode. This study offers new direction into the development of long-life and high-capacity Mg-ion batteries.

4 Experimental

4.1 Materials

Selenium disulfide (SeS_2 , 97%) was purchased from Shanghai Macklin Biochemical Co., Ltd. The electrolyte (DEGDME electrolyte including 0.5 M $\text{Mg}(\text{TFSI}_2)$) was purchased from Suzhou Dodochem Technology Co., Ltd. All reagents were used as received without further purification.

4.2 Synthesis of KB/S Composites

Ketjen Black (KB) and SeS_2 powder with the mass ratio of 5:4 were pyrolyzed at 255 °C for 12 h in the air. After cooled to room temperature, the KB/ SeS_2 composite material was obtained.

4.3 Synthesis of i -MXene ($\text{Mo}_{1.33}\text{C}$)

The $(\text{Mo}_{2/3}\text{Y}_{1/3})_2\text{AlC}$ i -MAX phases (where Y = Dy, Ho, Er, Tm, or Lu) were synthesized through press-free sintering. Mo powder (99.9% purity), intermediate Y_2Al_3 alloys (prepared by arc melting with rare-earth elemental chunks of 99.5% purity and aluminum metal of 99.95% purity), and graphite powder (99% purity) were ball-milled for 4 hours in a molar ratio of 4:1:2.4 ($\text{Mo}:\text{Y}_2\text{Al}_3:\text{C}$). The resulting mixture was placed in a graphite crucible and heated at 1400 °C for 1 hour with a temperature ramp rate of 5 °C min^{-1} , under a vacuum of about 5×10^{-2} Pa. After cooling to room temperature, the surface of the sintered products is polished to remove any oxide. The i -MXene $\text{Mo}_{1.33}\text{C}$ was obtained by etching the i -MAX phase $(\text{Mo}_{2/3}\text{Y}_{1/3})_2\text{AlC}$. To obtain the i -

MXene, 1 g of *i*-MAX phase ($\text{Mo}_{2/3}\text{Y}_{1/3}$)₂AlC powder was slowly added to 10 mL of 40% concentrated HF solution. The mixture was then transferred to a 50 mL polytetrafluoroethylene (PTFE)-lined stainless-steel autoclave and heated to 120 °C for 36 hours. After cooling to room temperature, the product was separated by centrifugation (8000 rpm for 6 minutes) and washed several times with 1 M hydrochloric acid (HCl) and deionized water until the supernatant was neutral. The precipitate was then dried under vacuum at 60 °C overnight to obtain multilayered *i*-MXene. Next, 10 mL of 40% TBAOH solution was added to a centrifuge tube containing 1 g of multilayered *i*-MXene, followed by ultrasonic treatment for 15 minutes. The mixture was then washed with alcohol and centrifuged to remove the TBAOH. Afterward, 20 mL of deionized water was added to the precipitate, and the suspension was treated by ultrasonic cleaner for an additional 15 minutes. The *i*-MXene suspension was obtained by centrifugation at 5000 rpm for 10 minutes. It should be noted that the *i*-MXene $\text{Mo}_{1.33}\text{C}$ can be obtained from any of the five ($\text{Mo}_{2/3}\text{Y}_{1/3}$)₂AlC powders, where Y = Dy, Ho, Er, Tm, or Lu.

4.4 Preparation of KB/SeS₂ electrodes

The KB/SeS₂ composite and guar gum were mixed in deionized water with a mass ratio of 9:1. Then the slurry was casted on a graphite foil followed by drying for 12 h in the air at 80 °C. The KB/SeS₂ electrodes were cut into disks with a diameter of 13.5 mm, the mass loading of the active material (SeS₂) was around 1 mg cm⁻². All full-cell capacities presented in this work are normalized to the mass of active SeS₂.

4.5 Preparation of SeS₂@*i*-MXene electrodes

The *i*-MXene and PVDF were mixed in NMP with a mass ratio of 9:1. Then the slurry was casted on KB/SeS₂ electrodes followed by drying for 12 h in the air at 80 °C. Then, a pressure of 10 MPa was applied for 3 minutes to fabricate the electrode, denoted as SeS₂@*i*-MXene. The mass loading of the *i*-MXene was around 1 mg cm⁻².

4.6 Preparation of S_x²⁻/Se_x²⁻ solution

Firstly, a KB/SeS₂ electrode with a high mass loading (5 mg cm⁻²) was prepared. The electrode was then tested in button cells at a current density of 0.1 A g⁻¹. Magnesium foil (thickness: 0.2 mm) without any modifications was used as the anode, and a glass fiber (GF) separator was placed between the anode and cathode. The electrolyte volume in each cell was 80 μL. The batteries were cycled ten times, after which the separators were immersed in 2 mL of DEGDME. After standing 10 min, the supernatant was collected as the S_x²⁻/Se_x²⁻ solution.

4.7 Magnesium-selenium disulfide battery assembly and electrochemical measurements

Button cells were assembled using graphite foil as current collectors. Magnesium foil (thickness: 0.2 mm), without any modifications, was employed as the anode. A glass fiber (GF) separator was placed between the anode and cathode, and the electrolyte volume in each cell was 80 μL.

The electrochemical performance of the assembled cells was evaluated using a multichannel electrochemical workstation (VMP3, Bio-Logic Science, France) and a Land battery testing system (LANHE).

4.8 Material characterization

X-ray diffraction (XRD, PANalytical B.V., X'Pert Pro, Netherlands) patterns were obtained to study the crystal structure. X-ray photoelectron spectroscopy (XPS, Thermo Scientific Escalab, ESCALAB 250 Xi, USA) was used to analyze the valence state of elements. Scanning electron microscopy (SEM) images were obtained on a field-emission scanning electron microscope (HITACHI, SU8010, Japan). Transmission electron microscopy (TEM, JEM-ARM200F, JEOL, Japan) measurements were used to analyze the morphology of the materials. Fourier transform infrared spectroscopy was recorded on a Fourier transform infrared spectrometer (VERTEX70, Bruker, Germany). Raman spectra were obtained on BWS465-532S, B&W Tek Inc., USA. with an excitation wavelength of 532 nm. Ex situ UV-vis adsorption spectra of electrolyte were probed by Evolution 220 at room temperature. Raman the UV spectroscopic studies were conducted to evaluate the dissolved species in the electrolyte. Briefly, when the battery discharged to the target voltage, the battery was disassembled, and the separator was immersed in 2 mL DEGDME. After standing, the supernatant was collected for spectroscopic analysis. For UV-vis spectroscopy, the baseline is calibrated using a mixture of 80 μL of 0.5 M Mg(TFSI)₂-DEGDME and 2 mL of DEGDME. N₂ adsorption and desorption isotherms were conducted by a N₂ physisorption analyzer at 77 K (Micromeritics, ASAP 2020).

4.9 Electrochemical measurement

For full-cell tests employing SeS₂- based cathodes, the galvanostatic charge-discharge voltage window was set to 0.2–2.4 V vs. Mg²⁺/Mg. Rate-performance measurements were performed at various current densities of 0.1, 0.2, 0.5, 1, and 2 A g⁻¹. Mg symmetric cells were cycled at a current density of 1 mA cm⁻² with a fixed areal capacity of 1 mAh cm⁻² for each Mg stripping/plating cycle.

4.10 Computational details

The DFT calculations are conducted using VASP, based on projector augmented wave (PAW) method. The PBE exchange-correlation functional within the generalized gradient approximation (GGA) is employed. The cutoff energy of the kinetic energy is 500 eV. The k-mesh in the Brillouin zone is 1×1×1 via Monkhorst-Pack method.

Acknowledgements

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Electronic Supplementary Material

Enhancing the cycling stability of Mg-SeS₂ batteries with an artificial electrode skin

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Supplementary Figures

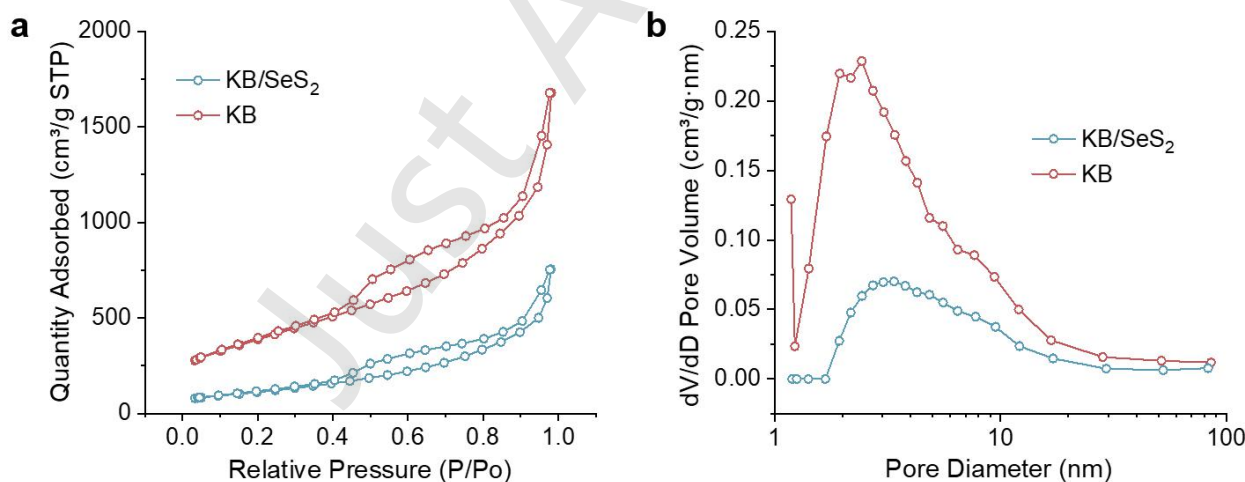


Fig. S1. (a) N₂ adsorption-desorption isotherms, and (b) the pore size distribution of KB and KB/SeS₂.

Ketjen black (KB) is a highly porous carbon black material. Such hierarchical porous architecture endows pristine KB with an extremely large specific surface area. After loading SeS₂, the KB/SeS₂ composite exhibits a significantly reduced specific surface area and decreased pore volume. The obvious attenuation of pore structure indicates that molten SeS₂ successfully infiltrates and fills the pores of KB. Therefore, we confirm that SeS₂ is uniformly incorporated within

the KB framework rather than simply physically mixed, achieving a homogeneous composite structure.

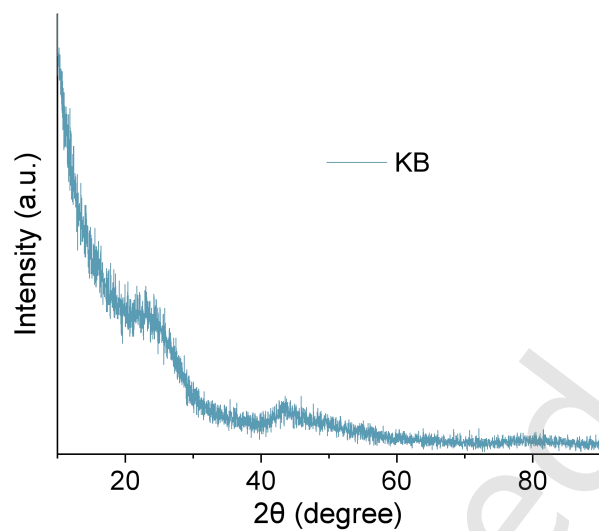


Fig. S2. XRD pattern of KB.

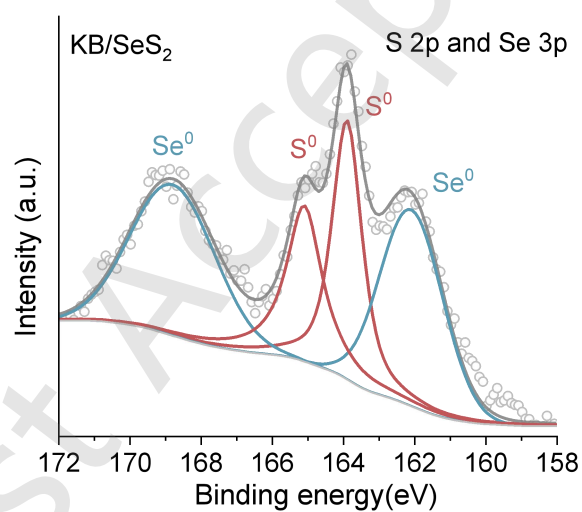


Fig. S3. XPS S 2p and Se 3p spectra of KB/SeS₂.

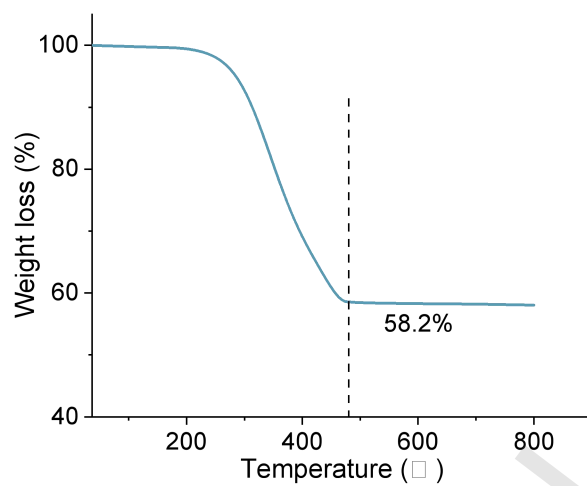


Fig. S4. TG curve of KB/SeS₂.

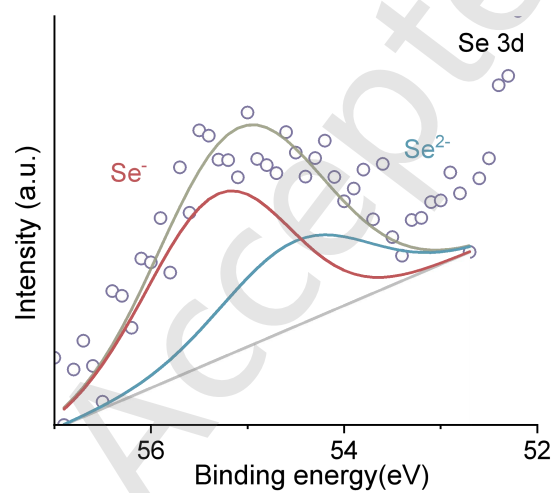


Fig. S5. XPS Se 3d spectra of Mg_{cycled}.

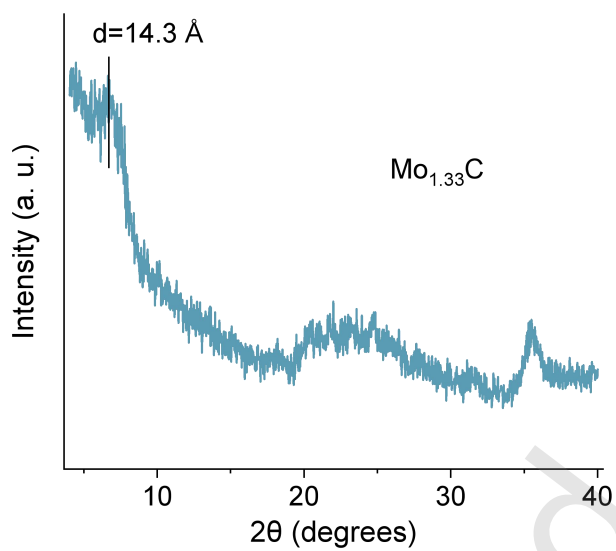


Fig. S6. XRD pattern of i -MXene $\text{Mo}_{1.33}\text{C}$.

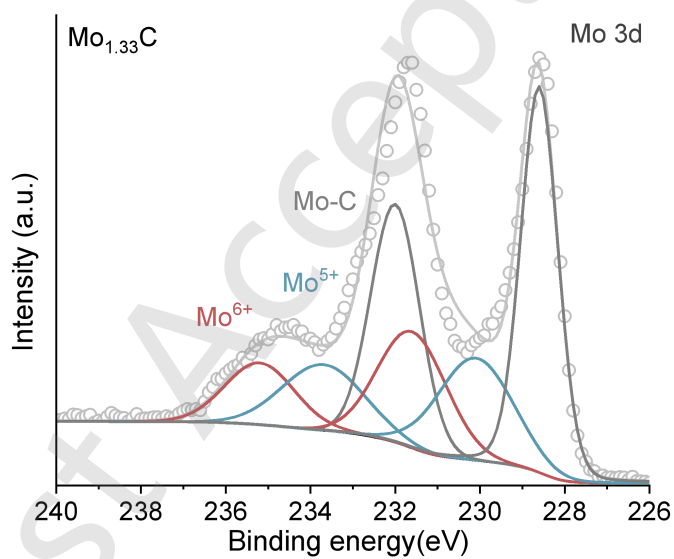


Fig. S7. XPS Mo 3d spectra of i -MXene $\text{Mo}_{1.33}\text{C}$.

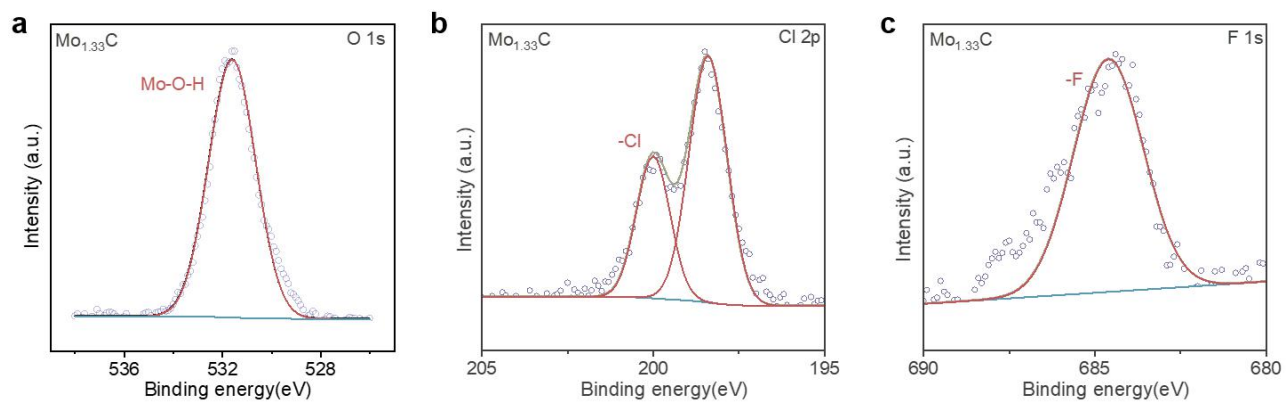


Fig. S8. XPS O 1s, F 1s, and Cl 2p spectra of i -MXene $\text{Mo}_{1.33}\text{C}$.

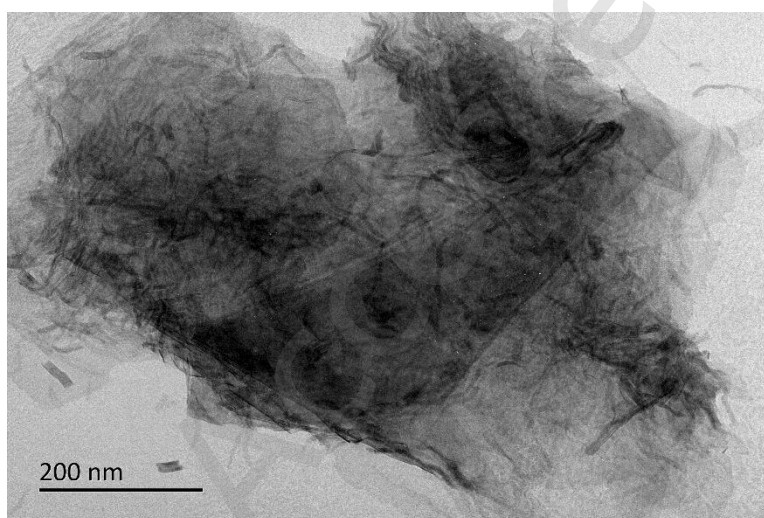


Fig. S9. TEM image of i -MXene $\text{Mo}_{1.33}\text{C}$.

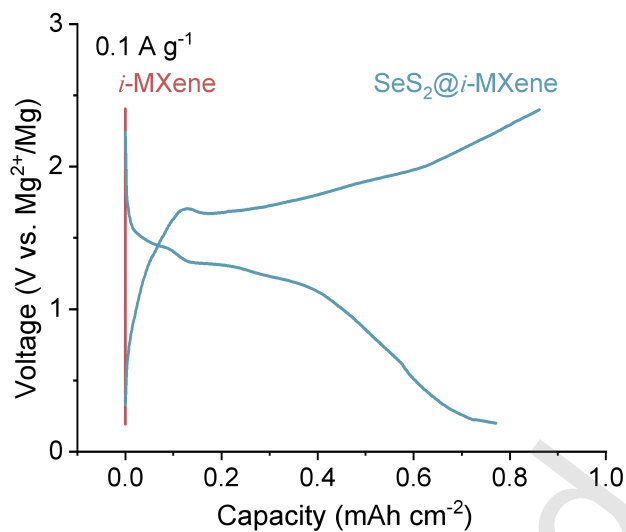


Fig. S10. The galvanostatic charge/discharge curves of Mg-SeS₂@*i*-MXene and *i*-MXene at a current density of 0.1 A g⁻¹.

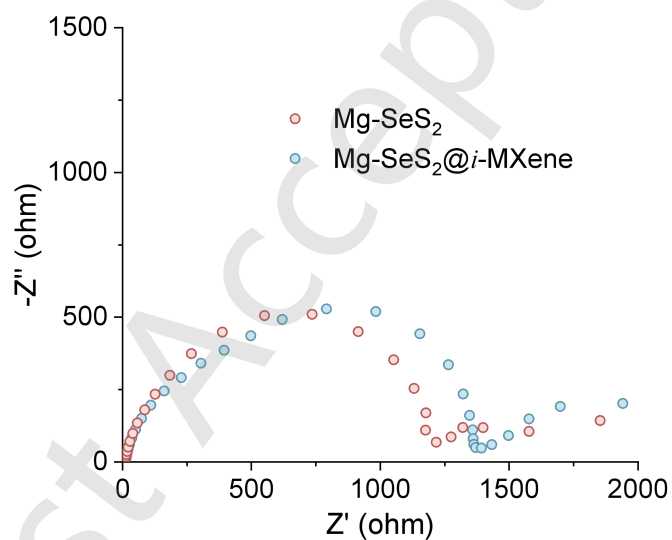


Fig. S11. EIS spectra of Mg-SeS₂ batteries and Mg-SeS₂@*i*-MXene batteries.

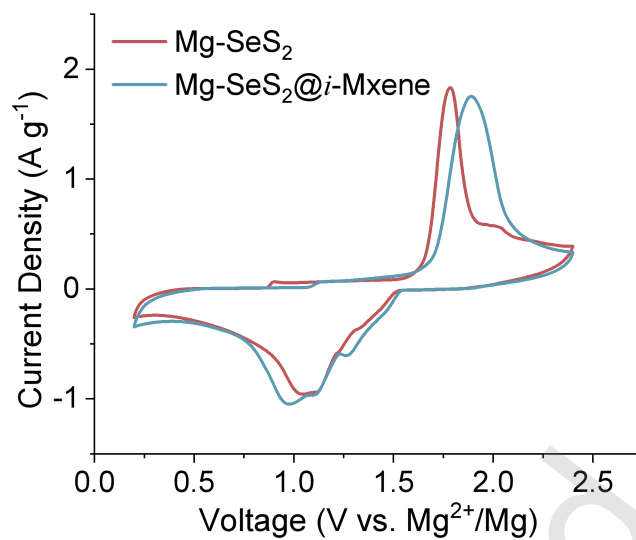


Fig. S12. CV curves of Mg-SeS₂ batteries and Mg-SeS₂@i-MXene batteries.

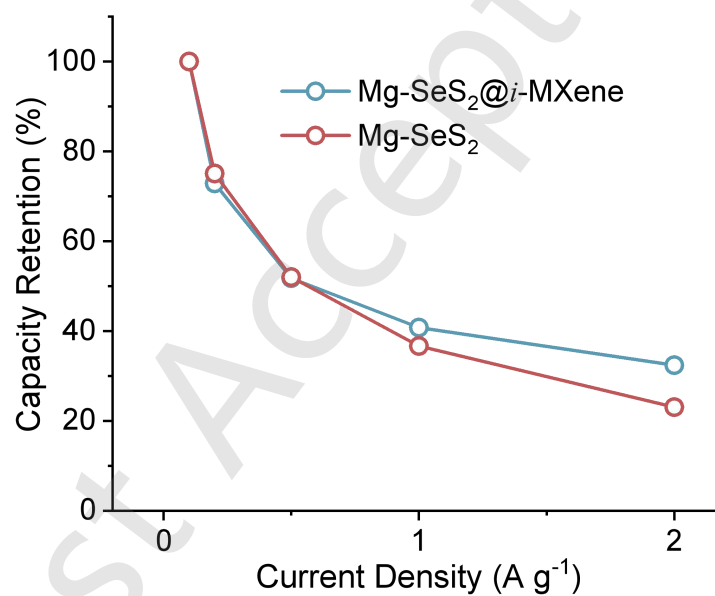


Fig. S13 Rate performance for Mg-SeS₂ batteries and Mg-SeS₂@i-MXene batteries.

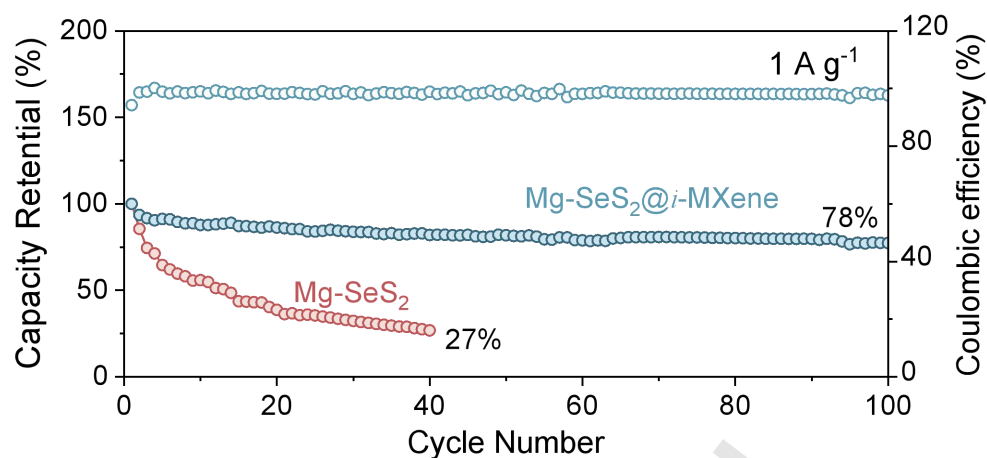


Fig. S14 Cyclic stability of Mg-SeS₂ batteries and Mg-SeS₂@i-MXene batteries at the current density of 1 A g⁻¹.

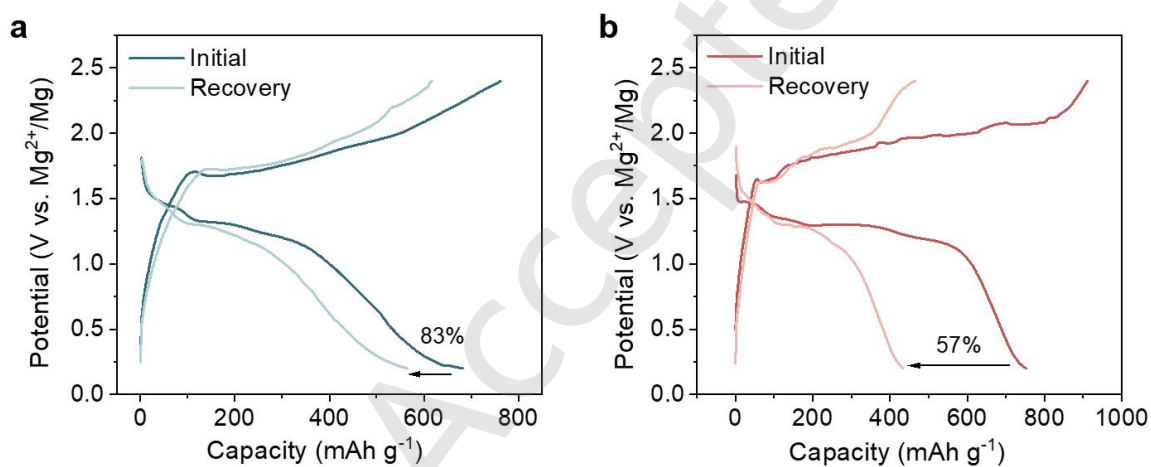


Fig. S15 Rate-recovery test for (a) Mg-SeS₂@i-MXene batteries and (b) Mg-SeS₂ batteries.

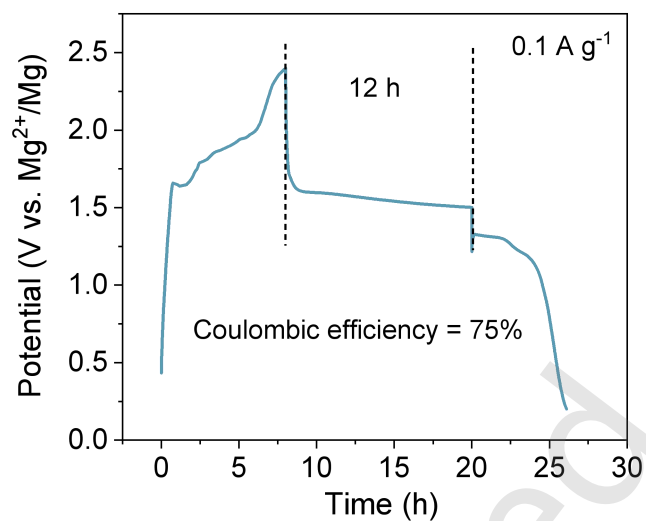


Fig. S16 Self-discharge measurement results in Mg-SeS₂@*i*-MXene batteries.

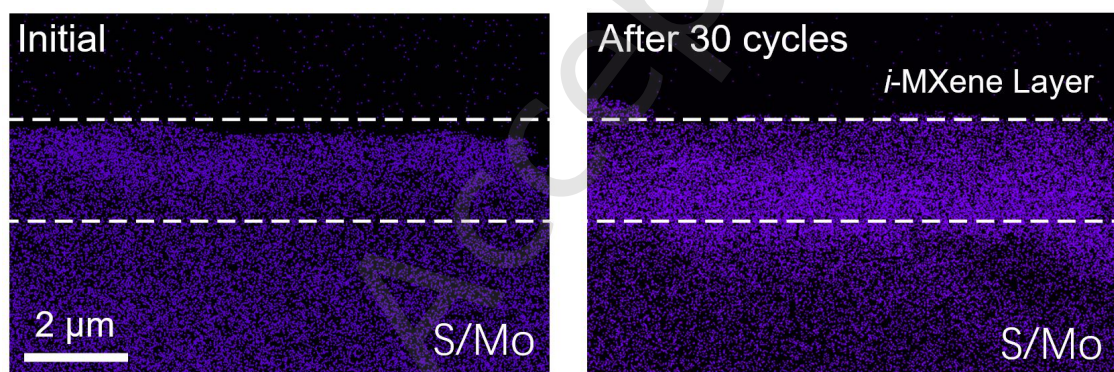


Fig. S17 Corresponding element mapping images for the SeS₂@*i*-MXene electrode cross-section before and after cycling.

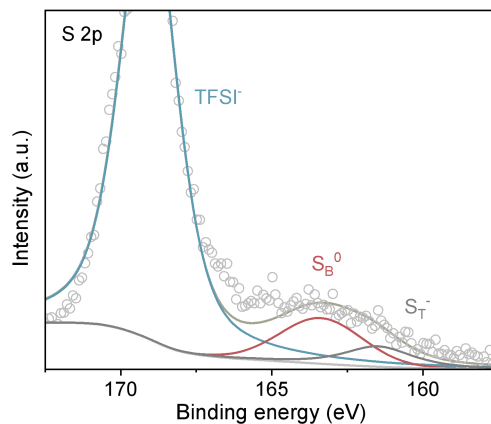


Fig. S18 XPS S 2p spectra for the *i*-MXene skin layer harvested from the electrode after 30 cycles.

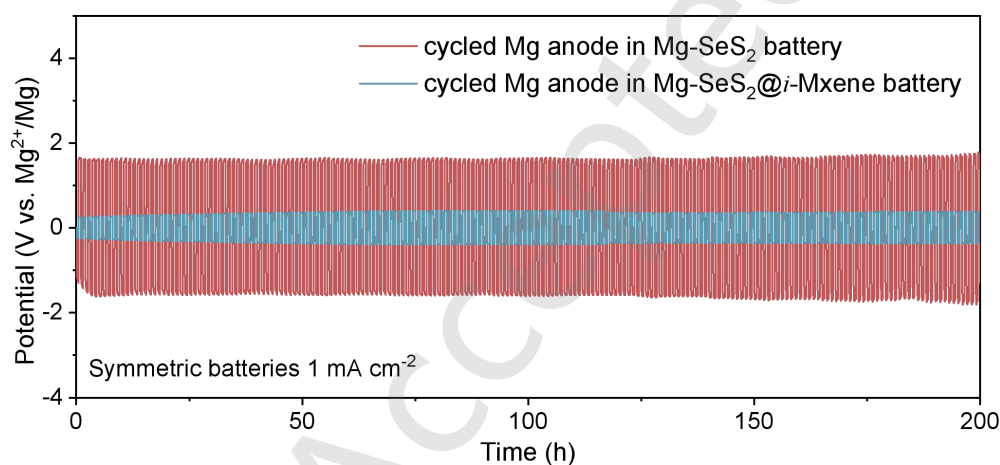


Fig. S19 Cycle test of the symmetric cells reassembled using cycled Mg anode in Mg-SeS₂ batteries and Mg-SeS₂@*i*-MXene batteries.

While the fresh Mg symmetric cell delivers an initial overpotential of 0.38 V, the pronounced degradation of full-cell performance upon cycling is strongly aggravated by shuttle-driven irreversible loss of active SeS₂ species and the consequent formation of detrimental SEI layers on the Mg anode. The *i*-MXene artificial electrode skin mitigates this degradation pathway by confining soluble chalcogen intermediates near the cathode side and suppressing S/Se-derived passivation on Mg anode.

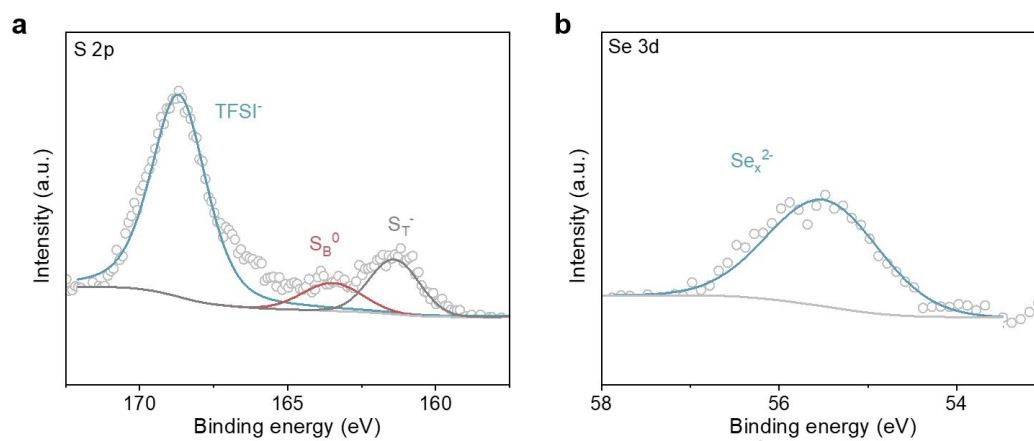


Fig. S20 S 2p and Se 3d spectra of *i*-MXene powder after the adsorption experiment.

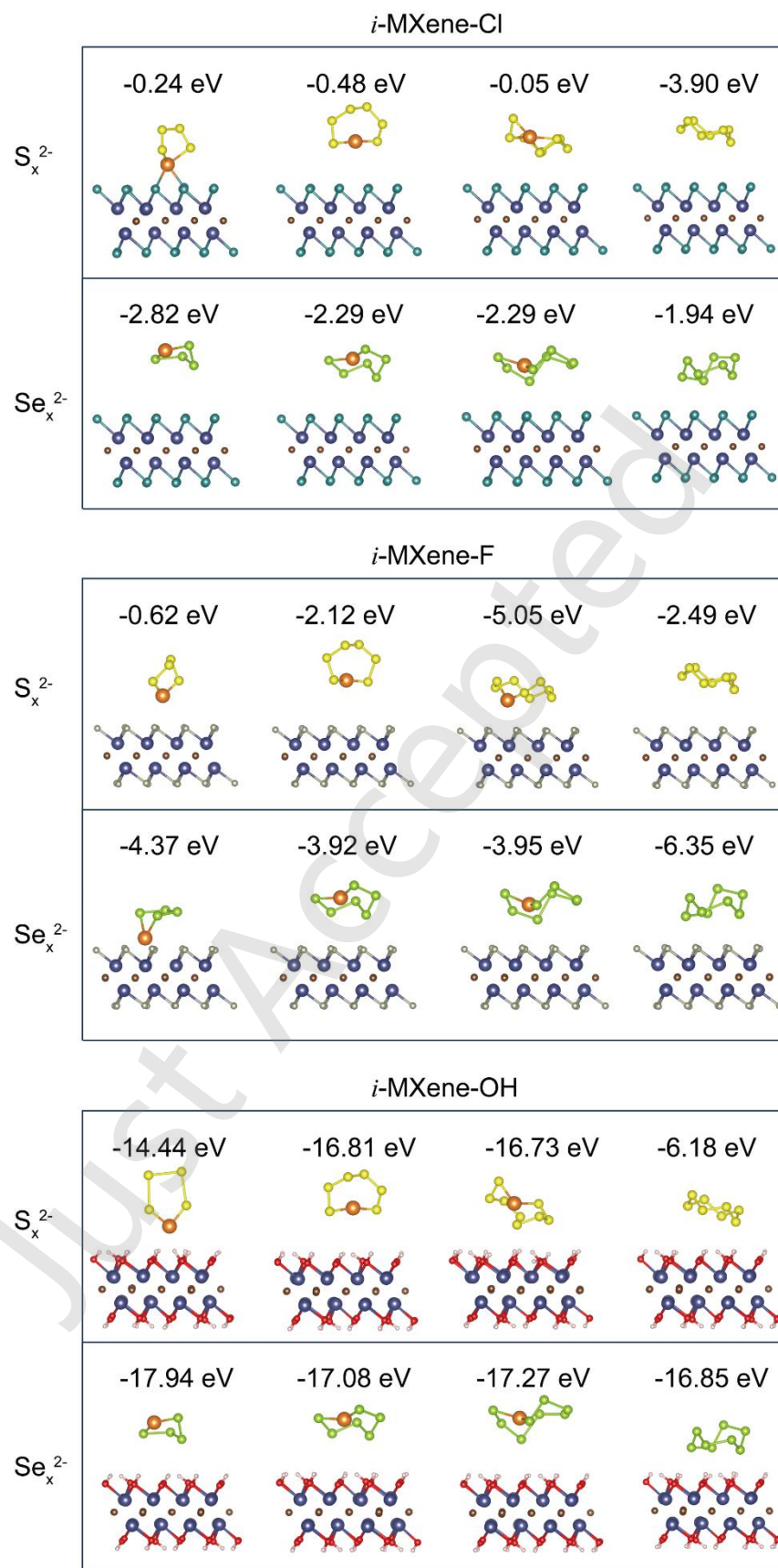


Fig. S21 The adsorption energy of S_x^{2-}/Se_x^{2-} on the *i*-MXene with different functional groups.

2. Supplementary Tables

Table S1 The Bonding Energy for the peaks in XPS spectra.

<i>Peak</i>	<i>Bonding Energy (eV)</i>
Mo ⁶⁺	235.2/231.7
Mo ⁵⁺	233.7/230
Mo-C	232/228.6
Mo-O-H	531.5
TFSI ⁻	168.8
S ⁰	168.9/162.1
S ²⁻	160
S _T ¹⁻	163.5
S _B ⁰	161.5
Se ⁰	165.1/163.9
Se ²⁻	54.2
Se _x ²⁻	55.2
F ⁻	684.6
Cl ⁻	200/198.4

Table S2 The initial capacity and capacity retention for KB/SeS₂ and SeS₂@*i*-MXene cathode at different current

<i>Cathode</i>	<i>Current Density (A g⁻¹)</i>	<i>Initial Capacity (mAh g⁻¹)</i>	<i>Cycle Number</i>	<i>Capacity Retention</i>
KB/SeS ₂	0.5	315	30	27%
SeS ₂ @ <i>i</i> -MXene	0.5	312	100	76%
KB/SeS ₂	1	234	40	27%
SeS ₂ @ <i>i</i> -MXene	1	246	100	78%
KB/SeS ₂	2	195	100	5%
SeS ₂ @ <i>i</i> -MXene	2	223	300	62%

density.