

Article

Coinage Metal Doping Engineering of Monolayer MoS₂ for Magnesium-Ion Battery Anodes: A First-Principles Study

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Abstract

Magnesium-ion batteries have attracted extensive attention due to their abundance, high safety, and superior volumetric energy density. However, their development remains constrained by the sluggish diffusion of Mg²⁺ ions and the limited magnesium storage capacity of electrode materials. In this work, we systematically investigate the Mg storage performance and underlying mechanisms of monolayer MoS₂ anodes substitutionally doped with Cu, Ag, and Au at a concentration of 4% on the Mo sublattice. The results reveal that all three dopants maintain the structural integrity of the two-dimensional MoS₂ framework after optimization while introducing localized electronic states near the Fermi level, thereby enhancing Mg adsorption. Compared with intrinsic MoS₂, the doped systems exhibit markedly improved Mg binding. Sequential adsorption calculations indicate that, at the investigated 4% substitution concentration, Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ can stably accommodate up to five Mg atoms, elevating the theoretical specific capacity to ~67 mAh/g while maintaining low open-circuit voltages during magnesium intercalation. Diffusion kinetics analysis further shows that Cu-MoS₂ possesses the lowest Mg migration barrier (0.25 eV), surpassing Ag-MoS₂ (0.38 eV) and Au-MoS₂ (0.61 eV). Considering both thermodynamic stability and ion transport kinetics, Cu-MoS₂ achieves an optimal balance among storage capacity, operating voltage, and diffusion performance, highlighting its promise as a high-performance anode material for magnesium-ion batteries.

Keywords: magnesium-ion batteries; monolayer MoS₂; coinage metal doping; density functional theory; anode materials

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1. Introduction

With the rapid expansion of grid-integrated renewable energy, electric mobility, and portable electronics, the development of next-generation electrochemical energy storage systems that simultaneously deliver high energy density, low cost, and superior safety has emerged as a central objective in energy materials research [1]. Although lithium-ion batteries have achieved widespread commercial success, the uneven distribution of lithium resources, fluctuations in material costs, and persistent safety concerns have motivated continued exploration of alternative energy storage technologies. Magnesium-based batteries have attracted considerable attention owing to their distinctive electrochemical characteristics. Metallic Mg offers several intrinsic advantages, including natural

abundance, relatively low cost, favorable chemical stability, and a high theoretical volumetric capacity [2–4]. In addition, Mg participates in a two-electron redox process, endowing magnesium-based energy storage systems with substantial promise for high-volumetric energy density applications [5]. Accordingly, the development of high-performance magnesium-ion batteries and their key electrode materials is of considerable significance for overcoming the resource and safety limitations associated with conventional lithium-based storage systems.

Despite these advantages, the advancement of magnesium-ion batteries remains constrained by a series of fundamental scientific and materials design challenges. On the one hand, Mg^{2+} possesses a high charge density and strong polarizing power, which generally give rise to pronounced electrostatic interactions with the host lattice of electrode materials [6,7]. Such interactions can lead to sluggish ion diffusion, limited insertion/extraction kinetics, and intensified structural responses during cycling [8]. On the other hand, in conventional Mg metal battery configurations, the Mg metal anode readily forms a passivating interphase in contact with common electrolytes, thereby obstructing reversible Mg deposition/stripping and imposing stringent requirements on both electrolyte formulations and electrode interfacial chemistry [9]. In contrast to the direct use of Mg metal anodes, the development of host-type anode materials capable of reversibly storing Mg provides an alternative strategy for mitigating interfacial compatibility issues associated with metallic Mg and for constructing magnesium-ion battery systems [10,11]. Nevertheless, an ideal host anode should not only exhibit stable Mg adsorption, but also combine a low operating potential, sufficient Mg storage capacity, excellent structural stability, and rapid Mg transport kinetics [12]. Therefore, the rational design of emerging anode materials that achieve an appropriate balance between adsorption thermodynamics and diffusion kinetics constitutes a critical challenge in advancing magnesium-ion batteries.

In recent years, two-dimensional (2D) materials have been regarded as promising electrode candidates for multivalent-ion batteries because of their high specific surface areas, abundant exposed active sites, shortened ion diffusion pathways, and tunable electronic structures [13,14]. Among them, layered molybdenum disulfide (MoS_2), a representative transition metal dichalcogenide, provides open two-dimensional surfaces for ion adsorption and migration [15]. Moreover, its local coordination environment and electronic state distribution can be modulated through phase engineering, defect regulation, heterostructure construction, and elemental doping [16–19]. Previous studies have demonstrated that layered MoS_2 can participate in Mg storage processes, and that the storage and migration behavior of Mg^{2+} can be effectively improved through regulation of solvated ions, structural phase reconstruction, or the construction of novel two-dimensional MoS_2 phases [20–22]. For example, theoretical investigations have shown that metallic B- MoS_2 and 1T- MoS_2 monolayers exhibit low open-circuit voltages, high Mg storage capacities, and favorable Mg migration characteristics when employed as anode materials for magnesium-ion batteries [23]. These findings indicate that tailoring the electronic structure and local atomic configuration represents an effective route toward enhancing the Mg storage performance of MoS_2 .

Although MoS_2 exhibits considerable potential for magnesium-ion storage, the Mg storage properties of pristine MoS_2 may remain limited by insufficient local electronic activity and relatively weak interactions between Mg and the substrate. For anode applications in particular, excessively weak Mg adsorption is unfavorable for initial magnesiation and stable Mg storage, whereas overly strong and highly localized interactions may result in substantial resistance to ion migration. Compared with strategies involving complete phase transformation or the construction of complex heterointerfaces, atomic-scale substitutional doping offers an attractive materials design approach for precisely regulating

the local electronic structure and surface adsorption characteristics of MoS₂ while preserving its parent two-dimensional framework [14,24,25]. Cu, Ag, and Au, as representative coinage metals, possess distinct atomic sizes, electronic configurations, and d-orbital characteristics. Their incorporation into the MoS₂ lattice is expected to generate new local M-S coordination environments and to regulate the charge distribution and orbital hybridization in the vicinity of Mg adsorption centers through dopant-associated electronic states. Existing studies have demonstrated that Cu doping can effectively enhance the magnesium storage performance of MoS₂-based materials. For example, Zhou et al. experimentally synthesized defect-rich Cu-doped 1T/2H MoS₂ nanosheets, in which the improved electrochemical performance originated from the combined effects of Cu incorporation, phase transition, defect engineering, and modulation of the interlayer structure [26]. Likewise, Alshareef et al. developed hierarchical nanocapsules composed of Cu-doped MoS₂ and hydrogen-substituted graphdiyne, where the enhanced Mg storage capability was attributed to the synergistic contributions of Cu doping, the carbonaceous heterointerface, the porous architecture, and nanoscale confinement [27]. While these studies substantiate the effectiveness of the Cu-doping strategy, they primarily focus on the experimental fabrication and electrochemical evaluation of systems involving a single coinage metal dopant and structurally complex electrodes. Consequently, the strong coupling among multiple structural factors obscures the intrinsic role of the dopant itself in governing Mg adsorption and diffusion. Moreover, systematic comparative investigations of the three group 11 coinage metals (Cu, Ag, and Au) under identical host structures, substitutional configurations, and doping concentrations remain scarce. How the identity of the coinage metal dopant modulates the local electronic structure, the thermodynamics of Mg adsorption, and the surface diffusion kinetics therefore remains an important open question warranting further investigation.

Motivated by these considerations, this work employs first-principles calculations to systematically investigate the potential of substitutionally Cu-, Ag-, and Au-doped MoS₂ monolayers as anode materials for magnesium-ion batteries. First, pristine and coinage metal-doped MoS₂ monolayer structures are constructed and optimized, and the effects of different dopants on the geometric configurations and electronic density of states of the substrates are analyzed. Subsequently, the preferred adsorption sites, adsorption stability, and successive adsorption behavior of Mg atoms on the different substrates are systematically examined, followed by an evaluation of the corresponding average open-circuit voltages and Mg storage capacities. Finally, Mg surface diffusion pathways and migration barriers are calculated to clarify how different dopant species regulate Mg migration behavior and the balance between adsorption thermodynamics and ion transport kinetics. This study clarifies the structure–property relationships governing Mg storage in coinage metal-doped MoS₂ and provides theoretical guidance for the rational design of two-dimensional chalcogenide-based anode materials for magnesium-ion batteries.

2. Computational Methods

2.1. First-Principles Calculation Parameters

All calculations were performed within the framework of density functional theory (DFT) using the Vienna Ab initio Simulation Package (VASP). The interactions between valence electrons and ionic cores were described by the projector-augmented wave (PAW) method, while the exchange correlation energy was treated using the Perdew–Burke–Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) [28–30]. The plane wave kinetic energy cutoff was set to 500 eV. For structural optimization and electronic structure calculations, the Brillouin zone was sampled using Monkhorst–Pack k-point meshes of $3 \times 3 \times 1$ and $5 \times 5 \times 1$, respectively [31]. To eliminate spurious interac-

tions between periodically repeated monolayers, a vacuum spacing of 20 Å was introduced along the direction perpendicular to the MoS₂ plane. During structural relaxation, the electronic self-consistent field convergence criterion was set to 10^{−5} eV, and all atoms were fully relaxed until the residual force on each atom was less than 0.01 eV Å^{−1}.

2.2. Construction of Structural Models

A 5 × 5 × 1 supercell was constructed on the basis of monolayer MoS₂. Pristine monolayer MoS₂ consists of two outer S atomic layers sandwiching a central Mo atomic layer, forming the characteristic S-Mo-S trilayer structure. To investigate the regulation of Mg storage properties in monolayer MoS₂ through coinage metal doping, one Mo atom in the supercell was substituted by a Cu, Ag, or Au atom, yielding the Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ systems, respectively. This substitution corresponds to a dopant concentration of 4% with respect to the Mo sublattice.

To examine Mg adsorption behavior, the adsorption stability of a single Mg atom at representative surface sites of pristine and doped MoS₂ monolayers was first evaluated, and the lowest-energy adsorption configuration was identified. Subsequently, the number of adsorbed Mg atoms was progressively increased to determine the energetically most favorable successive adsorption configurations at different Mg coverages. These optimized configurations were then employed to calculate the corresponding average open-circuit voltages and theoretical gravimetric capacities.

2.3. Calculation of Mg Adsorption Energy

The adsorption stability of Mg atoms on the substrate surface was evaluated using the adsorption energy (E_{ad}). For the adsorption of a single Mg atom, E_{ad} is defined as:

$$E_{ad} = E_{Mg@host} - E_{host} - E_{Mg} \quad (1)$$

where $E_{Mg@host}$ is the total energy of the substrate after Mg adsorption, E_{host} is the total energy of the Mg-free substrate, and E_{Mg} is the chemical potential of one Mg atom in bulk metallic Mg [32]. The host substrates considered herein include pristine MoS₂, Cu-MoS₂, Ag-MoS₂, and Au-MoS₂. A negative E_{ad} indicates that Mg adsorption is thermodynamically favorable, whereas a more negative value signifies stronger binding between Mg and the substrate.

For each substrate, all representative high-symmetry adsorption sites, including top, bridge and hollow positions, were initially considered. For the doped systems, additional adsorption sites located in the vicinity of and away from the dopant atom were also examined to account for the local structural asymmetry introduced by substitution. All candidate configurations were fully optimized, and the energetically most favorable adsorption structure was selected for subsequent analyses.

2.4. Average Open-Circuit Voltage and Theoretical Gravimetric Capacity

To evaluate the electrochemical performance of the different systems as anode materials for magnesium-ion batteries, the average open-circuit voltage during successive Mg adsorption was calculated. For the increase in Mg content from x_1 to x_2 , the average open-circuit voltage (V) is expressed as:

$$V = [E_{Mgx_2@host} + (x_2 - x_1)E_{Mg} - E_{Mgx_1@host}] / [2(x_2 - x_1)e] \quad (2)$$

where $E_{Mgx_2@host}$ and $E_{Mgx_1@host}$ are the total energies of the systems containing x_2 and x_1 adsorbed Mg atoms, respectively, and e is the elementary charge [33]. Because each Mg atom contributes two electrons during the electrochemical reaction, the transferred electron number is taken as 2. The Mg/Mg²⁺ redox couple is used as the reference electrode in the calculation of average open-circuit voltage. A positive voltage value indicates that Mg

adsorption on the host material is energetically favorable relative to the formation of bulk Mg metal.

When x Mg atoms are adsorbed in each computational model, the corresponding theoretical gravimetric capacity (C) can be calculated as:

$$C = 2xF / M_{host} \quad (3)$$

where F is the Faraday constant, taken as 96,485 C/mol, and M_{host} is the molar mass of the Mg-free substrate model. Because each Mg atom contributes two electrons, the electron transfer number is set to 2 [34]. This equation yields the theoretical gravimetric capacities, in mAh/g, of pristine and doped MoS₂ systems at different Mg coverages.

2.5. Calculation of Mg Migration Barrier

To investigate the migration kinetics of Mg atoms on differently doped MoS₂ monolayers, the climbing-image nudged elastic band (CI-NEB) method was employed to identify the minimum-energy migration pathways of Mg between adjacent stable adsorption sites [35]. The Mg diffusion barrier was defined as the energy difference between the highest-energy state along the migration pathway and the initial stable adsorption state. A lower diffusion barrier indicates more facile Mg migration across the electrode surface and is generally favorable for improving ion-transport kinetics and rate capability.

3. Results

3.1. Geometric and Electronic Structures

Figure 1 presents the optimized geometric structures of pristine, Cu-doped, Ag-doped, and Au-doped MoS₂ monolayers, including both top and side views. As shown in Figure 1a, the optimized pristine MoS₂ monolayer retains an intact hexagonal two-dimensional framework, indicating the favorable geometric stability of the constructed monolayer model [36]. To modulate the Mg storage behavior of monolayer MoS₂, one Mo site was substituted by a Cu, Ag, or Au atom, yielding the Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ models, respectively, as illustrated in Figure 1b–d. Following structural optimization, all three doped systems preserve the fundamental framework of the MoS₂ monolayer, without discernible lattice collapse, local bond cleavage, or severe out-of-plane structural distortion. These results demonstrate that substitutional doping with Cu, Ag, or Au introduces new local chemical environments while maintaining the integrity of the parent MoS₂ framework, thereby providing structurally reliable models for subsequent investigations of Mg adsorption and migration. Although geometry optimization confirms that the doped configurations are locally stable with respect to structural relaxation, it does not directly establish the thermodynamic feasibility of the substitutional doping process or guarantee experimental realizability. The dopant formation energies, kinetic pathways, and experimental investigations are required for a comprehensive evaluation of dopant incorporation stability. Nevertheless, previous experimental studies have demonstrated the successful synthesis of Cu-doped MoS₂ materials, suggesting that substitutional incorporation of coinage metal species into the MoS₂ framework can be experimentally achievable under appropriate synthesis conditions [26].

To further elucidate the influence of Cu, Ag, and Au doping on the electronic structure of monolayer MoS₂, the total density of states (TDOS) and projected density of states (PDOS) were calculated, as shown in Figure 2. For pristine monolayer MoS₂, a pronounced low-density-of-states region is observed near the Fermi level, indicative of its characteristic semiconducting electronic structure (Figure 2a). The valence-band region is predominantly contributed by Mo-d and S-p orbitals, with appreciable orbital overlap over a broad energy range, suggesting strong d-p hybridization between Mo and S atoms. By contrast,

the states near the conduction-band minimum are dominated by Mo-d orbitals, highlighting the decisive role of Mo-d electronic states in determining the frontier electronic structure of pristine MoS₂.

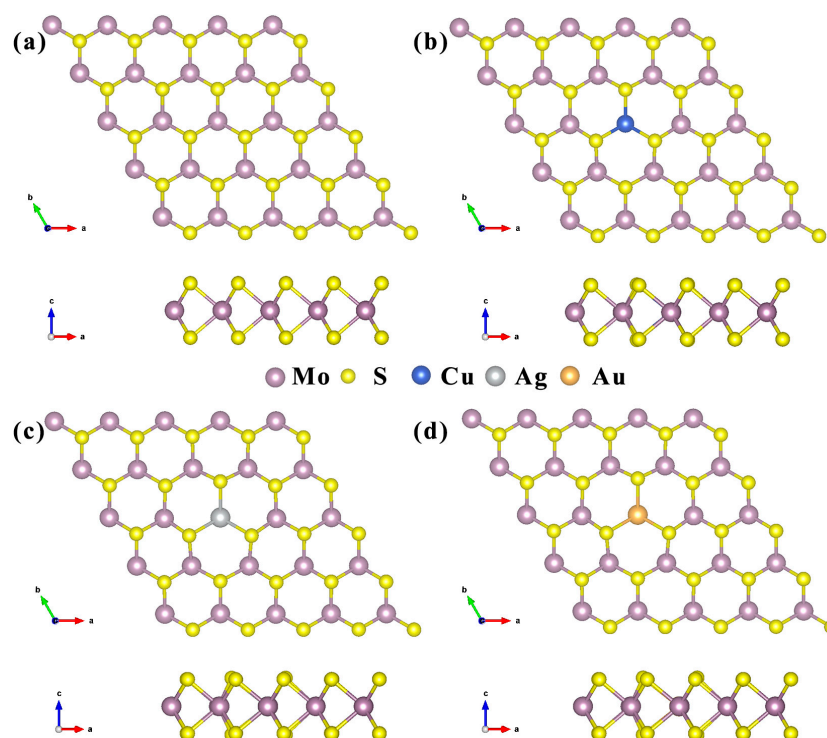


Figure 1. Top and side views of the optimized geometric structures of pristine and coinage metal-doped MoS₂ monolayers: (a) pristine MoS₂; (b) Cu-MoS₂; (c) Ag-MoS₂; and (d) Au-MoS₂. Purple, yellow, blue, silver-gray, and gold spheres represent Mo, S, Cu, Ag, and Au atoms, respectively.

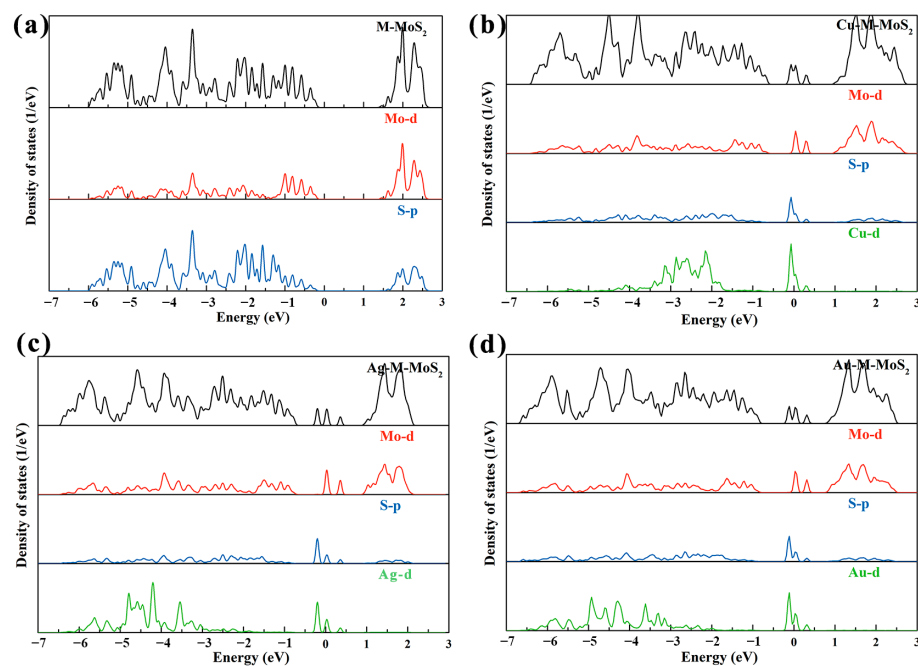


Figure 2. Total density of states and projected density of states of pristine and coinage metal-doped MoS₂ monolayers: (a) pristine MoS₂; (b) Cu-MoS₂; (c) Ag-MoS₂; and (d) Au-MoS₂.

Compared with the pristine system, the density-of-states distributions of Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ are substantially altered after substitutional doping. As shown in

Figure 2b–d, all three doped systems retain the principal electronic features derived from Mo-d and S-p orbitals, indicating that substitutional doping does not disrupt the fundamental bonding framework of the MoS₂ matrix. Meanwhile, the d orbitals of the dopant atoms introduce additional localized electronic states within the valence-band region and in the vicinity of the Fermi level, exhibiting varying degrees of energetic overlap with neighboring S-p and Mo-d orbitals. The emergence of these localized states suggests that coinage metal doping can effectively reconstruct the local electronic environment of surface-active regions in MoS₂. Overall, Cu, Ag, and Au doping preserve the essential electronic characteristics of the MoS₂ host while introducing dopant-associated localized states and promoting orbital interactions near the active centers. Such electronic structure modulation is expected to facilitate more stable Mg adsorption in the vicinity of the dopant sites.

3.2. Adsorption Behavior of a Single Mg Atom

The initial adsorption behavior of Mg atoms on the electrode surface provides an essential basis for evaluating the Mg storage capability of candidate anode materials [37]. To examine the effect of coinage metal doping on Mg adsorption stability, the adsorption behaviors of a single Mg atom at representative sites on pristine, Cu-doped, Ag-doped, and Au-doped MoS₂ monolayers were systematically investigated. The optimized adsorption configurations and corresponding adsorption energies are presented in Figure 3. It is worth noting that Figure 3 presents representative optimized adsorption configurations, while the most stable configuration among all investigated adsorption sites was selected for subsequent calculations.

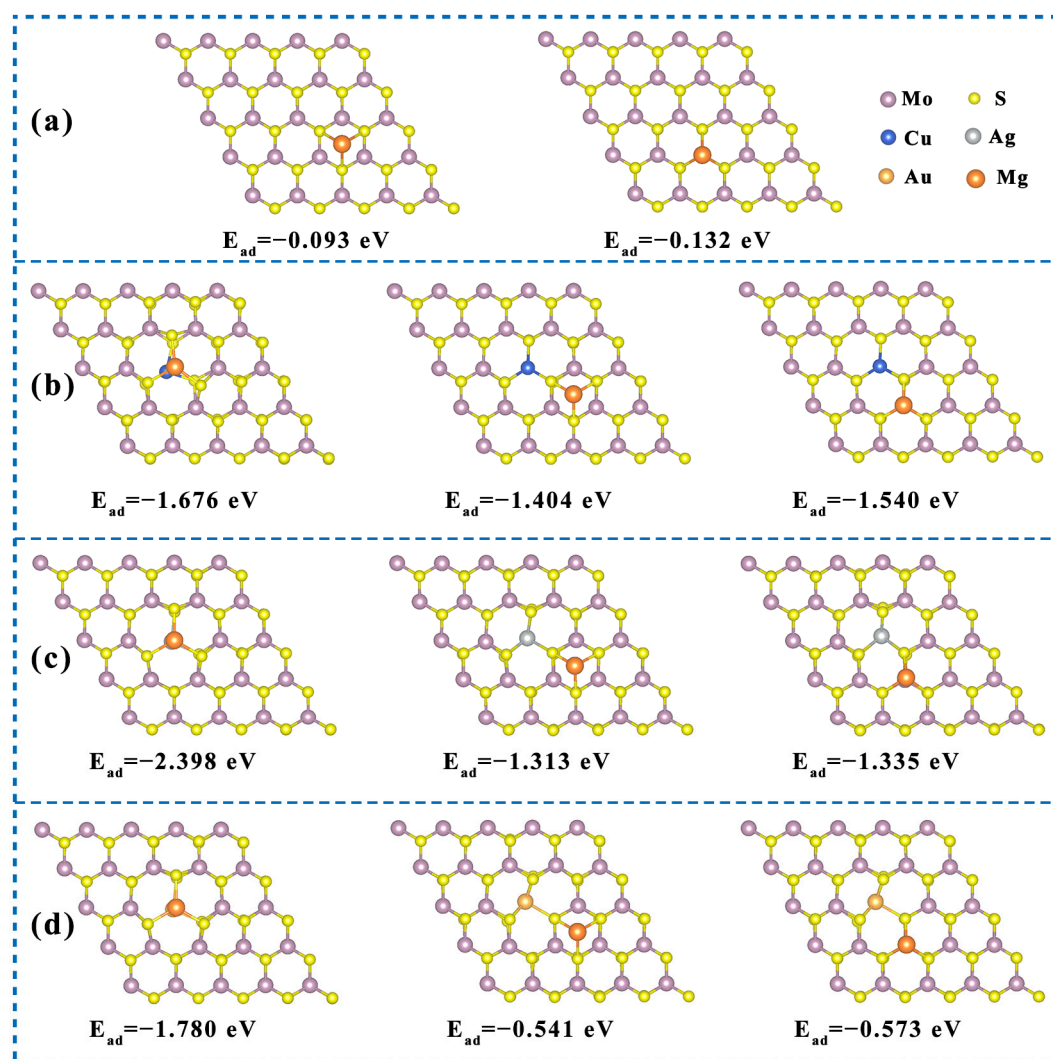


Figure 3. Optimized adsorption configurations and corresponding adsorption energies of Mg atoms at different adsorption sites on pristine and coinage metal-doped MoS₂ monolayers: (a) pristine MoS₂; (b) Cu-MoS₂; (c) Ag-MoS₂; and (d) Au-MoS₂. Purple, yellow, blue, silver-gray, gold, and orange spheres represent Mo, S, Cu, Ag, Au, and Mg atoms, respectively.

For pristine MoS₂, as shown in Figure 3a, the adsorption energies of Mg at the two representative adsorption sites are -0.093 and -0.132 eV, respectively. Both values are close to zero, indicating weak interactions between the Mg atom and the pristine MoS₂ surface, with no pronounced difference in stability between the investigated adsorption sites. These results suggest that unmodified monolayer MoS₂ lacks highly active sites capable of effectively stabilizing Mg atoms, resulting in relatively limited interfacial binding during the initial magnesiation process.

The introduction of Cu markedly enhances the adsorption stability of Mg. As shown in Figure 3b, the adsorption energies of Mg at three representative sites on Cu-MoS₂ are -1.676, -1.404, and -1.540 eV, respectively, all of which are substantially more negative than those obtained for pristine MoS₂. The most favorable adsorption configuration exhibits an adsorption energy of -1.676 eV, representing a decrease of 1.544 eV relative to the most stable configuration on pristine MoS₂. For Ag-MoS₂, the adsorption energies of Mg at the investigated sites are -2.398, -1.313, and -1.335 eV, respectively, as shown in Figure 3c. Notably, the most stable adsorption configuration delivers an adsorption energy of -2.398 eV, the lowest value among all systems considered. In the case of Au-MoS₂,

the adsorption energies of Mg at the three representative configurations are -1.780 , -0.541 , and -0.573 eV, respectively, as illustrated in Figure 3d.

Notably, for all three coinage metal-doped systems, the most favorable Mg adsorption configuration is located directly above the substitutional atom rather than the Mo top site. This preference originates from the modified local electronic environment induced by Cu, Ag, and Au substitution. The dopant atoms introduce localized d-orbital states near the Fermi level, which can enhance the interaction between Mg and the substrate through stronger orbital coupling. Since Mg tends to donate electrons upon adsorption, the electronically active dopant centers provide more favorable sites for charge transfer and stabilization of Mg compared with pristine Mo sites.

A comparison of the most stable Mg adsorption configurations across the four systems reveals that Ag-MoS₂ exhibits the strongest Mg adsorption, followed by Au-MoS₂ and Cu-MoS₂, whereas pristine MoS₂ shows by far the weakest affinity toward Mg. These results clearly indicate that substitutional doping with Cu, Ag, or Au creates localized active centers on the MoS₂ surface with substantially enhanced affinity for Mg, thereby improving the thermodynamic stability of the initial Mg adsorption process. Among the dopants investigated, Ag is particularly effective in strengthening initial Mg adsorption. By contrast, the surface activation induced by Au doping is highly localized, such that the adsorption stability of Mg is strongly dependent on its spatial proximity to the Au substitution site.

To further understand the electronic origin of the enhanced Mg adsorption induced by coinage metal doping, differential charge density and Bader charge analyses were performed for Mg adsorbed on pristine and doped MoS₂ monolayers (Figure 4). The charge transfer values indicate that Mg donates $0.76 e^-$ to pristine MoS₂, whereas much larger electron transfers of 1.65 , 1.63 , and $1.64 e^-$ occur for Cu-MoS₂, Ag-MoS₂, and Au-MoS₂, respectively. These results demonstrate that coinage metal doping significantly enhances the interfacial charge exchange between Mg and the MoS₂ substrate. The differential charge density distributions further reveal pronounced charge redistribution around the dopant centers and adjacent S atoms, confirming that Cu, Ag, and Au substitution creates electronically active regions for Mg adsorption.

It is worth noting that the adsorption energy does not solely depend on the amount of charge transfer. Although the Bader charge values of the three doped systems are comparable, Ag-MoS₂ exhibits the strongest Mg adsorption energy (-2.398 eV). This indicates that the adsorption strength is also governed by the local electronic configuration, orbital hybridization, and spatial interaction between Mg and the dopant-induced active center. The enhanced localized electronic states introduced by Ag doping provide stronger coupling with Mg, leading to a more favorable adsorption configuration.

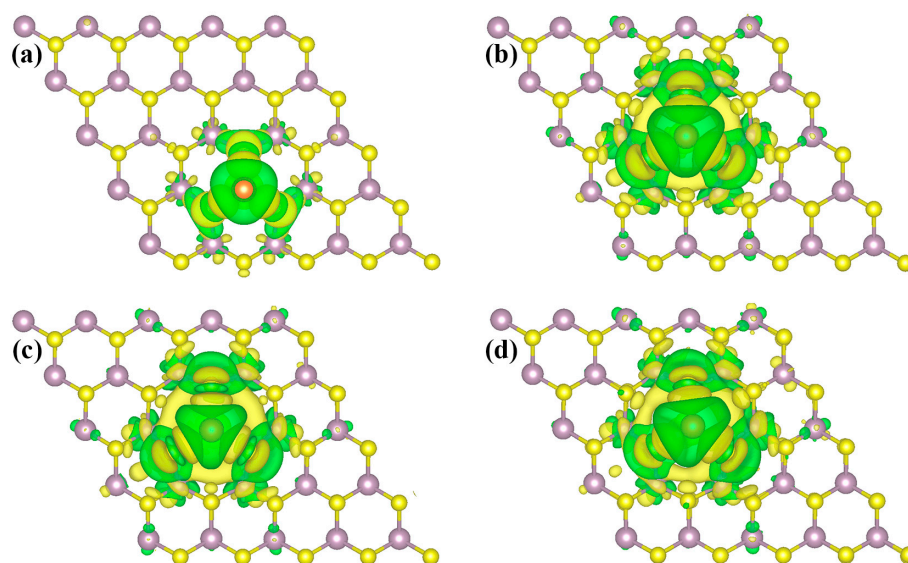


Figure 4. Differential charge density distributions of Mg adsorption on (a) pristine MoS₂, (b) Cu-MoS₂, (c) Ag-MoS₂, and (d) Au-MoS₂ monolayers. The green and yellow regions represent electron accumulation and electron depletion, respectively.

3.3. Structural Evolution and Mg Storage Capability During Successive Mg Adsorption

After identifying the most stable adsorption configuration for a single Mg atom, the successive adsorption behavior of increasing numbers of Mg atoms on Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ was further investigated to evaluate the structural stability and sustained Mg storage capability of the doped systems during progressive magnesiation. For each Mg loading level, multiple candidate configurations were considered, and the most energetically favorable structure was identified [38]. This procedure was continued until further Mg adsorption became thermodynamically unfavorable. Within the investigated 4% substitution models, pristine MoS₂ can accommodate only one Mg atom, whereas Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ can each stably accommodate up to five Mg atoms. Figure 5a–c presents the lowest-energy configurations of Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ after the successive adsorption of 1–5 Mg atoms, respectively, where structures I–V correspond to the optimized configurations at different Mg loading levels.

As shown in Figure 5, the first Mg atom in all three doped systems preferentially occupies a region adjacent to the dopant center. This feature is highly consistent with the single-Mg adsorption energy results, further confirming that Cu, Ag, and Au substitution creates localized active sites capable of preferentially capturing Mg atoms on the MoS₂ surface. As the number of adsorbed Mg atoms increases, additional Mg atoms progressively occupy stable adsorption sites surrounding the dopant center and in adjacent regions. This behavior indicates that the doped systems support a successive Mg storage process extending from strongly binding localized sites to additional accessible adsorption sites in the surrounding surface region.

Based on the definitions provided in the Computational Methods section, the voltage profiles and capacity variations in pristine, Cu-doped, Ag-doped, and Au-doped MoS₂ monolayers during successive Mg adsorption were further evaluated, as summarized in Figure 6. Pristine MoS₂ exhibits only a low initial voltage plateau of approximately 0.06 V during the early stage of Mg storage. This result is consistent with its weak single-Mg adsorption capability, indicating that pristine MoS₂ has limited ability to sustain stable Mg storage. In marked contrast, Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ can each stably adsorb five Mg atoms, corresponding to theoretical gravimetric capacities of approximately 67 mAh/g (4% substitution concentration). Because Cu, Ag, and Au possess different atomic

masses, slight differences in gravimetric capacity arise among the three doped systems at the same Mg loading level. By comparison, pristine MoS₂ can only marginally accommodate one Mg atom, affording a theoretical gravimetric capacity of merely approximately 13 mAh/g. These results further demonstrate that coinage metal doping substantially improves the Mg storage capability of monolayer MoS₂ relative to the pristine counterpart. The calculated capacity therefore represents a relative enhancement within the same computational framework rather than an intrinsic maximum capacity of coinage metal-substituted MoS₂. Because only one substitution concentration was examined, the dependence of active-site density and Mg storage capacity on dopant concentration cannot be determined from the present results.

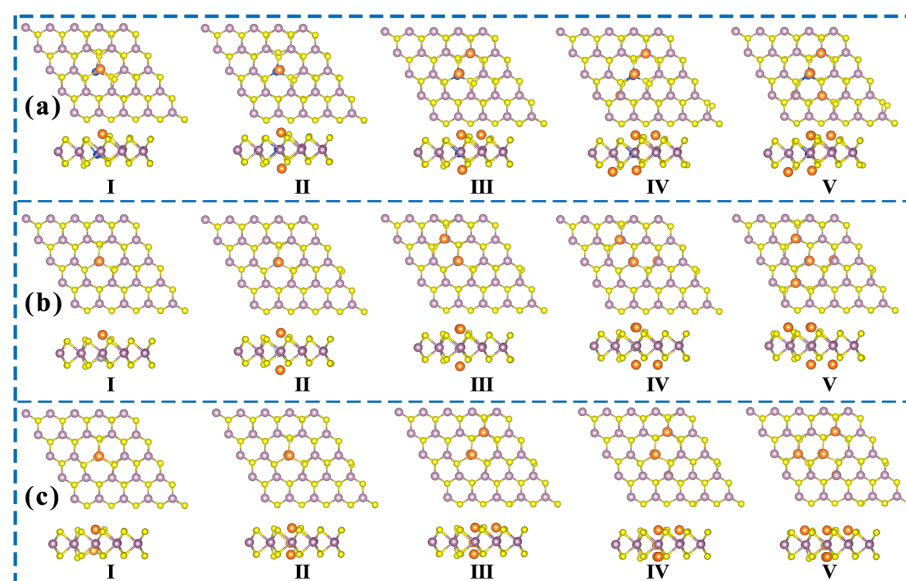


Figure 5. Top and side views of the sequential Mg adsorption configurations on coinage metal-doped MoS₂ monolayers: (a) Cu-MoS₂; (b) Ag-MoS₂; and (c) Au-MoS₂. Structures I–V correspond to the lowest-energy configurations after the sequential adsorption of 1–5 Mg atoms, respectively.

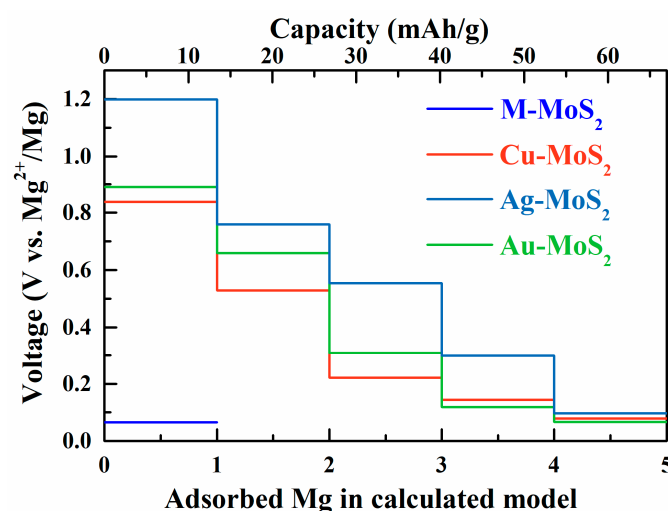


Figure 6. Average open-circuit voltage profiles and corresponding Mg storage capacities of pristine, Cu-doped, Ag-doped, and Au-doped MoS₂ monolayers during successive Mg adsorption.

As revealed by the calculated voltage profiles in Figure 6, the voltages of all three doped systems decrease stepwise with increasing Mg loading. This behavior can be at-

tributed to the sequential occupation of adsorption sites with progressively weaker binding strengths [39]. During the initial stage of magnesiation, the most strongly binding active sites in the vicinity of the dopant centers are occupied preferentially. As Mg coverage increases, subsequent Mg atoms are accommodated at relatively weaker adsorption sites, while the progressively intensified repulsive interactions among adsorbed Mg atoms further reduce the energetic favorability of additional adsorption. Cu-MoS₂ exhibits an average open-circuit voltage of 0.36 V. Among the three doped systems, Ag-MoS₂ delivers the highest overall voltage response, with an average voltage of 0.58 V during successive Mg adsorption, whereas Au-MoS₂ displays an average voltage of 0.41 V. Taken together, the enhanced Mg storage capacities relative to pristine MoS₂ and the comparatively low operating voltages suggest that the three coinage metal-doped MoS₂ monolayers are promising anode candidates for magnesium-ion batteries.

3.4. Surface Diffusion Behavior and Migration Kinetics of Mg

In addition to thermodynamic stability and capacity characteristics, the mobility of Mg on the anode surface is another critical factor governing rate capability and charge/discharge kinetics [40–42]. A lower migration barrier enables Mg atoms to move more readily between adjacent stable adsorption sites, thereby facilitating a rapid ionic response during high-rate electrochemical operation. Previous first-principles calculations have reported that the Mg diffusion barrier on pristine monolayer MoS₂ is approximately 0.48 eV [36]. Therefore, the present work focuses on revealing how different coinage metal dopants regulate Mg migration behavior relative to this reported pristine system. Accordingly, the diffusion pathways and corresponding energy variations in Mg on Cu-MoS₂, Ag-MoS₂, and Au-MoS₂ were further investigated, as summarized in Figure 7.

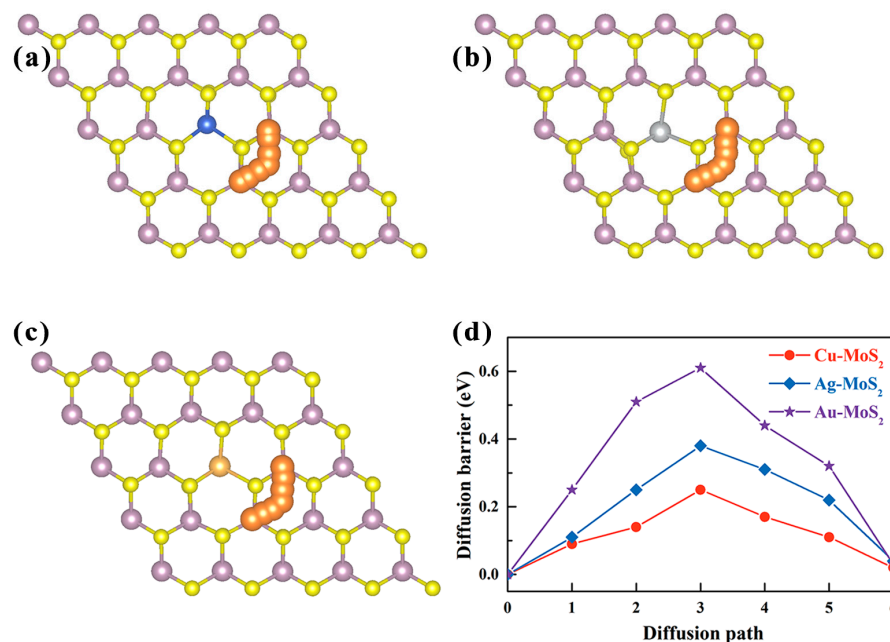


Figure 7. Diffusion pathways of Mg atoms on coinage metal-doped MoS₂ monolayers and the corresponding diffusion energy barriers: (a) Cu-MoS₂; (b) Ag-MoS₂; (c) Au-MoS₂; and (d) relative energy profiles along the Mg migration pathways.

Figure 7a–c presents representative migration pathways of Mg on the surfaces of Cu-MoS₂, Ag-MoS₂, and Au-MoS₂, respectively, while the corresponding diffusion energy profiles are shown in Figure 7d. On the Cu-MoS₂ surface, Mg exhibits a diffusion barrier of approximately 0.25 eV, the lowest among the three doped systems. When considered together with its favorable Mg adsorption stability, this result indicates that Cu doping

not only substantially strengthens Mg adsorption on the MoS₂ surface, but also avoids imposing a pronounced kinetic penalty on Mg migration.

For Ag-MoS₂, the diffusion barrier of Mg is approximately 0.38 eV, which is higher than that on Cu-MoS₂ but remains relatively modest. Given that Ag-MoS₂ exhibits the strongest Mg adsorption among the investigated systems, the moderately increased diffusion barrier can be attributed to the enhanced local stabilization of Mg in the vicinity of the Ag dopant. Migration from such a strongly binding site to an adjacent adsorption position necessarily involves overcoming a larger energetic fluctuation. Nevertheless, the diffusion barrier of Ag-MoS₂ does not increase to a level expected to severely impede Mg migration, suggesting that this system retains acceptable ion transport capability while providing pronounced thermodynamic stabilization of adsorbed Mg.

By comparison, Au-MoS₂ exhibits the highest Mg diffusion barrier, approximately 0.61 eV. Although Au doping effectively enhances Mg adsorption, the relatively large migration barrier indicates that Mg transport on the Au-MoS₂ surface is more kinetically restricted. This behavior is consistent with the highly localized adsorption enhancement induced by Au substitution: Mg atoms are strongly stabilized in the vicinity of the Au site, but consequently experience greater difficulty escaping from the resulting local potential well and migrating toward neighboring positions. Therefore, although Au-MoS₂ possesses favorable Mg adsorption stability, its capability for rapid ion transport may be inferior to those of Cu-MoS₂ and Ag-MoS₂.

It should be noted that the Mg adsorption strength does not directly determine the diffusion kinetics. The diffusion barrier is governed by the energy difference between the initial adsorption state and the transition state along the migration pathway. Although Ag-MoS₂ exhibits the strongest Mg adsorption, the migration barrier remains moderate because the Mg binding environment around Ag does not excessively restrict surface migration. In contrast, Au doping generates more localized electronic interactions, resulting in a deeper adsorption potential well around the Au center and a larger energetic penalty during Mg migration. Cu-MoS₂ achieves the lowest diffusion barrier because it provides sufficient Mg stabilization while maintaining a relatively smooth migration energy landscape, indicating a more favorable balance between adsorption thermodynamics and transport kinetics.

Overall, coinage metal substitutional doping modifies the local geometric configuration and electronic state distribution of monolayer MoS₂, thereby generating surface-active centers with enhanced affinity toward Mg and markedly improving its Mg storage behavior. Among the investigated dopants, Ag is the most effective in strengthening Mg adsorption stability and increasing the thermodynamic driving force for Mg storage. Cu doping, by contrast, achieves a more favorable balance among stable Mg adsorption, low operating voltage, and rapid Mg diffusion. Although Au doping enhances Mg adsorption, its comparatively high migration barrier may limit high-rate charge/discharge performance. On the basis of these results, Cu-MoS₂ can be regarded as a promising anode candidate that combines favorable thermodynamic stability with efficient Mg transport kinetics, whereas Ag-MoS₂ exhibits distinctive advantages in reinforcing interfacial Mg immobilization. These findings demonstrate that the rational selection of coinage metal dopants provides an effective strategy for tailoring the Mg storage properties of two-dimensional MoS₂-based anode materials and offers theoretical guidance for the design of high-performance magnesium-ion battery anodes.

4. Conclusions

In this study, first-principles calculations were employed to systematically investigate the regulation of Mg storage properties in monolayer MoS₂ through substitutional doping with Cu, Ag, and Au. Structural optimization results demonstrate that all three

coinage metal-doped models maintain the structural integrity of the two-dimensional MoS₂ framework after relaxation, suggesting their local structural stability for subsequent Mg storage investigations. Electronic structure analyses reveal that the d orbitals of the dopant atoms introduce localized electronic states in the vicinity of the Fermi level and enhance orbital hybridization within the active regions, thereby providing an electronic origin for the strengthened interactions between Mg and the substrate. Compared with the weak Mg adsorption exhibited by pristine MoS₂, Cu, Ag, and Au doping substantially improve Mg adsorption stability. In particular, Ag-MoS₂ delivers the most negative adsorption energy of −2.398 eV, indicative of the strongest affinity toward Mg among the investigated systems. Successive adsorption and voltage analyses further show that each doped system (4% substitution concentration) can stably accommodate up to five Mg atoms while maintaining structural integrity throughout the adsorption process. Relative to pristine MoS₂, which exhibits highly limited Mg storage capability, substitution with Cu, Ag, or Au at a 4% concentration increases the theoretical gravimetric capacity to approximately 67 mAh/g within the investigated models. Diffusion kinetics calculations reveal that Cu-MoS₂ possesses the lowest Mg migration barrier, only 0.25 eV, outperforming Ag-MoS₂ and Au-MoS₂ in terms of Mg transport kinetics. Overall, Ag doping is particularly advantageous for strengthening Mg adsorption stability, whereas Cu doping affords a more favorable balance among adsorption capability, operating potential, and ion-migration kinetics. These results identify Cu-MoS₂ as a promising anode candidate for magnesium-ion batteries and demonstrate that coinage metal substitution is an effective strategy for modulating the Mg storage behavior of two-dimensional MoS₂.

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References

1. Xiao, J.; Adelstein, N.; Bi, Y.; Bian, W.; Cabana, J.; Cobb, C.L.; Cui, Y.; Dillon, S.J.; Doeff, M.M.; Islam, S.M.; et al. Assessing cathode–electrolyte interphases in batteries. *Nat. Energy* **2024**, *9*, 1463–1473. <https://doi.org/10.1038/s41560-024-01639-y>.
2. Yan, X.; Luo, S.-H.; Liu, Q.; Sun, Q.; Yan, S.-X.; Wang, Q.; Zhang, Y.; Liu, X. Insertion-type cathode materials in magnesium ion batteries: Research progress and application potential. *Mater. Today Energy* **2025**, *53*, 102001. <https://doi.org/10.1016/j.mtener.2025.102001>.
3. Tian, H.J.; Gao, T.; Li, X.G.; Wang, X.; Luo, C.; Fan, X.; Yang, C.; Suo, L.; Ma, Z.; Han, W.; et al. High power rechargeable magnesium/iodine battery chemistry. *Nat. Commun.* **2017**, *8*, 14083. <https://doi.org/10.1038/ncomms14083>.

4. Chen, C.; Liang, Z.; Tao, D.; Zhang, D.; Cao, Y.; Xu, F.; Li, T. Unveiling the Interlayer–Intralayer Cooperative Diffusion Mechanism in Bimetallic Layered Cathodes for Rechargeable Magnesium Batteries. *ACS Nano* **2025**, *19*, 34180–34191. <https://doi.org/10.1021/acsnano.5c10711>.
5. Kotobuki, M.; Yan, B.; Lu, L. Recent progress on cathode materials for rechargeable magnesium batteries. *Energy Storage Mater.* **2023**, *54*, 227–253. <https://doi.org/10.1016/j.ensm.2022.10.034>.
6. Zhang, X.; Li, D.; Ruan, Q.; Liu, L.; Wang, B.; Xiong, F.; Huang, C.; Chu, P.K. Vanadium-based cathode materials for rechargeable magnesium batteries. *Mater. Today Energy* **2023**, *32*, 101232. <https://doi.org/10.1016/j.mtener.2022.101232>.
7. Lei, X.; Liang, X.; Yang, R.; Zhang, F.; Wang, C.; Lee, C.S.; Tang, Y. Rational design strategy of novel energy storage systems: Toward high-performance rechargeable magnesium batteries. *Small* **2022**, *18*, e2200418. <https://doi.org/10.1002/smll.202200418>.
8. Xu, H.; He, X.; Li, Y.; Guo, Q.; Sun, X.; Xie, X.; Liu, L.; Laine, R.M.; Zou, J.; Feng, X.; et al. Reassessing Electrolyte Design for Non-Aqueous Magnesium Batteries: Atomistic Structures and Performance Optimization. *Adv. Mater.* **2025**, *38*, e14224. <https://doi.org/10.1002/adma.202514224>.
9. Radi, M.; Purkait, T.; Tchitcheкова, D.S.; Goñi, A.R.; Markowski, R.; Bodin, C.; Courrèges, C.; Dedryvère, R.; Ponrouch, A. A Comprehensive Study on the Parameters Affecting Magnesium Plating/Stripping Kinetics in Rechargeable Mg Batteries. *Adv. Energy Mater.* **2024**, *14*, 2401587. <https://doi.org/10.1002/aenm.202401587>.
10. Miao, X.; Chen, Z.; Wang, N.; Nuli, Y.; Wang, J.; Yang, J.; Hirano, S.-I. Electrospun V₂MoO₈ as a cathode material for rechargeable batteries with Mg metal anode. *Nano Energy* **2017**, *34*, 26–35. <https://doi.org/10.1016/j.nanoen.2017.02.014>.
11. Ma, N.; Wang, T.; Li, N.; Li, Y.; Fan, J. New phases of MBenes M₂B (M = Sc, Ti, and V) as high-capacity electrode materials for rechargeable magnesium ion batteries. *Appl. Surf. Sci.* **2022**, *571*, 151275. <https://doi.org/10.1016/j.apsusc.2021.151275>.
12. Mousavian, S.M.H.; Bautin, V.A. Rechargeable magnesium batteries: Overcoming challenges for high-efficiency energy applications. *J. Energy Storage* **2025**, *126*, 117079. <https://doi.org/10.1016/j.est.2025.117079>.
13. Li, S.; He, W.; Adelhelm, P.; Xu, C. Recent Progress in Interlayer Engineering of Layered Materials for High-Performance Magnesium Ion Batteries. *ACS Appl. Mater. Interfaces* **2025**, *17*, 46505–46520. <https://doi.org/10.1021/acsaem.8b00843>.
14. Mukherjee, S.; Singh, G. Two-Dimensional Anode Materials for Non-lithium Metal-Ion Batteries. *ACS Appl. Energy Mater.* **2019**, *2*, 932–955. <https://doi.org/10.1021/acsaem.8b00843>.
15. Hu, X.L.; Zhang, W.; Liu, X.X.; Mei, Y.; Huang, Y. Nanostructured Mo-based electrode materials for electrochemical energy storage. *Chem. Soc. Rev.* **2015**, *44*, 2376–2404. <https://doi.org/10.1039/c4cs00350k>.
16. Zhang, Y.X.; Kuwahara, Y.; Mori, K.; Louis, C.; Yamashita, H. Hybrid phase 1T/2H-MoS₂ with controllable 1T concentration and its promoted hydrogen evolution reaction. *Nanoscale* **2020**, *12*, 11908–11915. <https://doi.org/10.1039/d0nr02525a>.
17. Chu, K.; Liu, Y.; Li, Y.; Guo, Y.; Tian, Y. Two-dimensional (2D)/2D interface engineering of a MoS₂/C₃N₄ heterostructure for promoted electrocatalytic nitrogen fixation. *ACS Appl. Mater. Interfaces* **2020**, *12*, 7081–7090. <https://doi.org/10.1021/acsaem.8b00843>.
18. Ding, W.; Hu, L.; Dai, J.M.; Tang, X.; Wei, R.; Sheng, Z.; Liang, C.; Shao, D.; Song, W.; Liu, Q.; et al. Highly ambient-stable 1T-MoS₂ and 1T-WS₂ by hydrothermal synthesis under high magnetic fields. *ACS Nano* **2019**, *13*, 1694–1702. <https://doi.org/10.1021/acsnano.8b07744>.
19. He, X.; Wang, R.; Yin, H.; Zhang, Y.; Chen, W.; Huang, S. 1T-MoS₂ monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. *Appl. Surf. Sci.* **2022**, *584*, 152537. <https://doi.org/10.1016/j.apsusc.2022.152537>.
20. Li, L.; Hu, Z.; Zhao, S.; Chou, S.-L. Alkali and alkaline-earth metal ion–solvent co-intercalation reactions in nonaqueous rechargeable batteries. *Chem. Sci.* **2021**, *12*, 15206–15218. <https://doi.org/10.1039/d1sc04202e>.
21. Wang, M.; Ye, H.; Vasudevan, V.; Medhekar, N.V. Enhancing kinetic and electrochemical performance of layered MoS₂ cathodes with interlayer expansion for Mg-ion batteries. *J. Power Sources* **2022**, *542*, 231722. <https://doi.org/10.1016/j.jpowsour.2022.231722>.
22. Li, B.; Li, Z.; Chen, H.; Zhang, X.; Wu, S.; Xu, H.; Yao, Y.; Li, Y.; Li, X.; Hu, Z.; et al. Li⁺ additive accelerated structural transformation of MoS₂ cathodes for performance-enhancing rechargeable Mg²⁺ batteries. *Mater. Today Energy* **2022**, *27*, 101047. <https://doi.org/10.1016/j.mtener.2022.101047>.
23. Wu, D.; Yang, B.; Zhang, S.; Ruckenstein, E.; Chen, H. Reshaping two-dimensional MoS₂ for superior magnesium-ion battery anodes. *J. Colloid Interface Sci.* **2021**, *597*, 401–408. <https://doi.org/10.1016/j.jcis.2021.04.002>.
24. Ding, Y.; Yan, Z.; Wang, G.; Sang, H.; Xu, Z.; Li, W. Regulating the Oxygen Vacancy and Electronic Structure of NiCo Layered Double Hydroxides by Molybdenum Doping for High-Power Hybrid Supercapacitors. *Small* **2024**, *20*, e2306382. <https://doi.org/10.1002/smll.202306382>.

25. Kim, K.S.; Shinde, N.M.; Yun, J.M.; Kim, K.H. Sulfur and phosphorus co-doped nickel-cobalt layered double hydroxides for enhancing electrochemical reactivity and supercapacitor performance. *RSC Adv.* **2021**, *11*, 12449–12459. <https://doi.org/10.1039/d1ra00424g>.
26. Xu, A.; Liu, Y.; Wang, J.; Wang, Y.; Jiang, F.; Zhou, Y. Highly defective and conductive Cu-doped 1T/2H-MoS₂ nanosheets as high-capacity cathode materials for enhanced magnesium-ion storage. *Inorg. Chem. Front.* **2024**, *11*, 7831–7842. <https://doi.org/10.1039/d4qi02064b>.
27. Zhuo, S.; Huang, G.; Sougrat, R.; Guo, J.; Wei, N.; Shi, L.; Li, R.; Liang, H.; Shi, Y.; Zhang, Q.; et al. Hierarchical Nanocapsules of Cu-Doped MoS₂@H-Substituted Graphdiyne for Magnesium Storage. *ACS Nano* **2022**, *16*, 3955–3964. <https://doi.org/10.1021/acsnano.1c09405>.
28. Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996**, *77*, 3865–3868. <https://doi.org/10.1103/PhysRevLett.77.3865>.
29. Kresse, G.; Furthmüller, J. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Phys. Rev. B* **1996**, *54*, 11169–11186. <https://doi.org/10.1103/PhysRevB.54.11169>.
30. Kresse, G.; Joubert, D. From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B* **1999**, *59*, 1758–1775.
31. Monkhorst, H.J.; Pack, J.D. Special points for Brillouin-zone integrations. *Phys. Rev. B* **1976**, *13*, 5188–5192. <https://doi.org/10.1103/PhysRevB.13.5188>.
32. Wang, Z.W.; Li, W.L.; Zheng, Y.P.; Yang, Z.; Zhang, J. How does the active site in the MoSe₂ surface affect its electrochemical performance as anode material for metal-ion batteries? *Appl. Surf. Sci.* **2020**, *526*, 146637. <https://doi.org/10.1016/j.apsusc.2020.146637>.
33. Zhu, J.J.; Gandi, A.N.; Schwingenschlogl, U. Potential of B/Al-doped silicene electrodes in Na/K-ion batteries. *Adv. Theory Simul.* **2018**, *1*, 1800017. <https://doi.org/10.1002/adts.201800017>.
34. Wang, D.; Liu, Y.; Meng, X.; Wei, Y.; Zhao, Y.; Pang, Q.; Chen, G. Two-dimensional VS₂ monolayers as potential anode materials for lithium-ion batteries and beyond: First-principles calculations. *J. Mater. Chem. A* **2017**, *5*, 21370–21377. <https://doi.org/10.1039/C7TA06944H>.
35. Henkelman, G.; Uberuaga, B.P.; Jonsson, H. A climbing image nudged elastic band method for finding saddle points and minimum energy paths. *J. Chem. Phys.* **2000**, *113*, 9901–9904. <https://doi.org/10.1063/1.1329672>.
36. Yang, S.; Li, D.; Zhang, T.; Tao, Z.; Chen, J. First-principles study of zigzag MoS₂ nanoribbon as a promising cathode material for rechargeable Mg batteries. *J. Phys. Chem. C* **2012**, *116*, 1307–1312. <https://doi.org/10.1021/jp2097026>.
37. Shuai, J.; Yoo, H.D.; Liang, Y.; Li, Y.; Yao, Y.; Grabow, L.C. Density functional theory study of Li, Na, and Mg intercalation and diffusion in MoS₂ with controlled interlayer spacing. *Mater. Res. Express* **2016**, *3*, 064001. <https://doi.org/10.1088/2053-1591/3/6/064001>.
38. Yang, J.; Wang, J.; Wang, X.; Dong, X.; Zhu, L.; Zeng, W.; Wang, J.; Pan, F. First-principles prediction of layered MoO₂ and MoOSe as promising cathode materials for magnesium ion batteries. *Nanotechnology* **2021**, *32*, 495405. <https://doi.org/10.1088/1361-6528/ac21f2>.
39. Urban, A.; Seo, D.-H.; Ceder, G. Computational understanding of Li-ion batteries. *Npj Comput. Mater.* **2016**, *2*, 16002. <https://doi.org/10.1038/npjcompumats.2016.2>.
40. Kulish, V.V.; Koch, D.; Manzhos, S. Ab initio study of Li, Mg and Al insertion into rutile VO₂: Fast diffusion and enhanced voltages for multivalent batteries. *Phys. Chem. Chem. Phys.* **2017**, *19*, 22538–22545. <https://doi.org/10.1039/C7CP04360K>.
41. Xu, K.; Liao, N.; Zhang, M.; Xue, W. Atomic-scale investigation of enhanced lithium, sodium and magnesium storage performance from defects in MoS₂/Graphene heterostructure. *Nanoscale* **2020**, *12*, 7098–7108. <https://doi.org/10.1039/C9NR09352D>.
42. Zhao, S.J.; Kang, W.; Xue, J.M. The potential application of phosphorene as an anode material in Li-ion batteries. *J. Mater. Chem. A* **2014**, *2*, 19046–19052. <https://doi.org/10.1039/C4TA04368E>.

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