

Review

Energetic and dynamic principles of potassium electrodeposition in potassium metal batteries

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CONTEXT & SCALE The pursuit of high-energy, low-cost, and sustainable energy storage has renewed interest in potassium metal batteries (PMBs) that offer natural abundance, low material cost, and favorable electrochemical properties. However, uncontrolled potassium (K) dendrite growth remains a critical barrier to the practical deployment of PMBs. Although studies have investigated materials and interfacial engineering strategies to mitigate K dendrite formation, the fundamental mechanisms that govern K nucleation and early-stage growth, which ultimately drive dendrite development, are still not fully understood.

This review addresses this knowledge gap by establishing a theoretical framework to describe K electrodeposition from both thermodynamic and kinetic perspectives. Key interfacial parameters, including contact angle, surface energy, interfacial energy, and binding energy, are systematically analyzed to explain nucleation behavior and inform substrate design. The combined effects of binding and interfacial energies are also explored in alloying systems to demonstrate how K nucleation can be selectively promoted and controlled. In parallel, solid-electrolyte interphase (SEI) is examined as a dynamic and functional interface. Its mechanical strength and ionic conductivity are identified as critical factors that influence interfacial stability and deposition morphology. Strategies for enhancing SEI performance through materials and electrolyte engineering are reviewed in detail.

By integrating energetic principles with recent advances in interfacial chemistry and materials design, this review presents a principle-based framework for suppressing dendrite formation and achieving reversible K metal plating. It also outlines future research directions, including *in situ* and *operando* characterization, rational electrolyte formulation, and multiscale modeling, to improve understanding of SEI evolution and electrodeposition dynamics. Overall, this work bridges theoretical understanding and practical strategies, providing guidance for the rational design of stable K metal anodes and accelerating the development of scalable, high-performance PMBs.

SUMMARY

Potassium metal batteries offer a sustainable and cost-effective solution for high-energy storage applications. However, uncontrolled potassium dendrite growth remains a major obstacle to achieving long-term stability. In this review, we provide a holistic overview by establishing a theoretical framework for potassium nucleation and early-stage growth, identifying key factors that influence stable electrodeposition. We discuss representative materials and substrate design strategies that address these factors and emphasize the importance of several energetic parameters, including contact angle, surface energy, interfacial energy, binding energy, and combined binding/interfacial energies. These descriptors offer insight into the thermodynamic and kinetic processes governing potassium deposition. In addition, we explore the dynamic role of the solid-electrolyte interphase, particularly its mechanical properties and ionic conductivity, which critically impact deposition behavior. Finally, we outline future research directions toward a principle-driven, knowledge-based approach for regulating potassium electrodeposition, aiming to lay the groundwork for the practical development of next-generation potassium metal batteries.



INTRODUCTION

Alkali metal batteries have come into the research spotlight in the quest for high-energy batteries to combat carbon emissions and achieve the net-zero goal.^{1–3} Utilizing alkali metal anodes (Li, Na, or K) can result in an over two-fold gravimetric energy improvement compared with conventional ion-insertion anodes, with the gravimetric capacities of 3,861 (Li), 1,165 (Na), and 678 mAh g^{−1} (K) versus 372 mAh g^{−1} for LiC₆, 250–350 mAh g^{−1} for Na in hard carbons and 279 mAh g^{−1} for KC₈. Despite the high gravimetric capacity of Li metal anodes, the scarcity of Li, constituting merely 0.0017 wt.% of the Earth's crust, along with its rapid consumption, uneven global distribution, and supply-chain challenges, is raising concerns about long-term sustainability and feasibility. Emerging Na and K metal anodes are excellent alternatives to Li metal anodes, owing to their abundance (2.36 wt.% for Na and 2.09 wt.% for K) and exemption from geographic and geopolitical restrictions. Compared with Na, K holds the advantages of a lower electrodeposition potential by 0.23 V in propylene carbonate (PC) solvents and a smaller Stokes radius (3.6 Å for K ions versus 4.6 Å for Na ions), which can translate to a higher cell voltage and better rate capability.⁴ These favorable attributes establish potassium metal batteries (PMBs) as a promising candidate for next-generation energy storage systems.

K electrodeposition is undoubtedly critical to the successful operation of PMBs. However, it is highly susceptible to uncontrolled K nucleation and growth, leading to high nucleation overpotential and locally amplified K-ion flux. These effects contribute to K dendrite formation, which can penetrate the separator and potentially cause thermal runaway or even fires. While sizeable K-ion insertion in the cathode also presents challenges, ongoing progress in potassium-ion batteries (PIBs) has led to the development and optimization of numerous K cathode materials, many of which can be readily adapted for PMBs. Excellent summaries of K cathodes are available in previous reviews.^{5,6} By contrast, K dendrite growth at the K metal anode remains a major unsolved issue. Furthermore, K electrodeposition is intricately influenced by the solid-electrolyte interphase (SEI), whose formation, stability, and dynamic evolution throughout cycling are not yet fully understood. Although recent studies indicate progress toward unraveling these complexities, the interplay between K electrodeposition and SEI appears extremely complex.⁷ Achieving long-term stable K metal plating and stripping is essential not only for the practical use of PMBs but also for enabling a near-stoichiometric anode-to-cathode ratio.⁸ Minimizing excess K metal usage is imperative for enhancing safety and mitigating risks associated with PMB operation.⁹

Research on stabilizing K electrodeposition has progressed in recent years, with many studies focusing on improving overall K metal anode performance. While various strategies have been proposed, the fundamental mechanisms underlying these approaches are not always well established. As the development of K metal anodes is still in its early stages, the emergence of diverse strategies, even sometimes demonstrating effectiveness unexpectedly, reflects the exploratory nature of the field. To facilitate systematic progress, a holistic perspective on K electrodeposition, combined with a comprehensive understanding of K nucleation and early-stage growth mechanisms, is essential.

Developing these fundamental insights will help integrate seemingly independent studies and establish a structured framework for designing effective strategies, ultimately driving further advancements in PMBs.

This review endeavors to bridge fundamental principles with recent advances in achieving stable K electrodeposition. It outlines key factors derived from theoretical frameworks, progressing from contact angle, surface energy, and interfacial energy to binding energy, then to the combined effects of binding and interfacial energies, and further to the role of the SEI, reflecting the evolving understanding of K electrodeposition. Additionally, it delves into innovative material and substrate design strategies anchored in these key factors, emphasizing established knowledge while identifying open questions to guide future research on K metal anodes. From a comprehensive yet distinctive perspective, this review seeks to catalyze broader discussions on K electrodeposition and its profound implications for the future of PMBs.

K NUCLEATION AND GROWTH DURING ELECTRODEPOSITION

Nucleation is a critical process to initiate the formation of new crystals, specifically K crystals in this context. During PMB charging, K metal deposition takes place at the anode surface, either metallic K or the current collector, as shown in Figure 1. Under an applied potential, K ions are released from the cathode material, traverse the cathode-electrolyte interphase (CEI), become solvated by the electrolyte molecules, diffuse toward the anode, shed their solvation shell at the interface of the electrolyte and SEI, traverse the SEI, and form K adatoms (adsorbed atoms) at the SEI/anode interface. Before nucleation can occur, the K adatoms adhere to the anode surface, creating an adsorption layer. Once a sufficient number of adatoms converge at a particular location on the anode surface, they coalesce to form a critical cluster or nucleus, which serves as the foundational point for the subsequent growth of K crystals.¹⁰

For a cluster to stabilize and grow, it must first overcome the nucleation barrier, the energy required for K adatoms to transition from a disordered state to an orderly crystalline structure on the anode surface. This barrier is influenced by factors such as applied voltage, anode surface properties, electrolyte composition, and the presence of impurities or additives.¹¹ Once the critical cluster stabilizes, growth occurs through the sequential addition of K atoms, which adsorb onto the anode surface, diffuse, and integrate into the growing crystal. The growth mode varies depending on the nucleation scenario and may follow any of the mechanisms in Figure 2B, including the Frank-van der Merwe, Stranski-Krastanov, or Volmer-Weber models.¹² The Frank-van der Merwe mode (layer-by-layer growth) involves smooth monolayer growth under strong substrate adhesion (adhesion energy > cohesion energy) and lattice matching. The Stranski-Krastanov mode (layer-plus-island growth) begins with wetting layer(s) formation due to adhesion dominance, transitioning to three-dimensional (3D) islands as strain from lattice mismatch overcomes adhesion. The Volmer-Weber mode (island growth) features the formation of 3D islands without a wetting layer (cohesion energy > adhesion energy), common in weakly interacting systems.^{11,15}

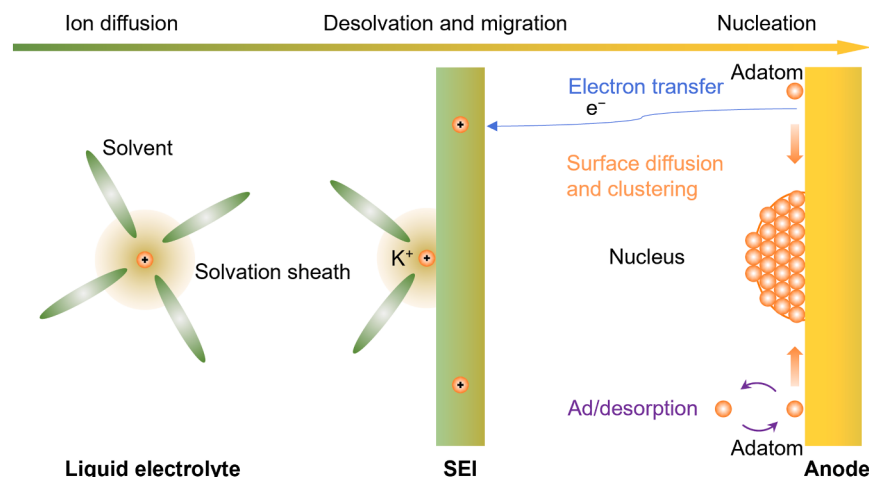


Figure 1. Schematic illustration of K nucleation during electrodeposition

The diffusion of K ions within the electrolyte is depicted, followed by their desolvation at the electrolyte/SEI interface. Subsequently, these ions traverse the SEI, acquire electrons, and emerge as adatoms at the SEI/anode interface. The adatoms then undergo surface diffusion across the anode surface, coalescing into clusters. When the clusters reach a sufficient size, they crystallize to create a nucleus that serves as the foundation for further growth. By contrast, smaller clusters lack the stability to preserve their structure and consequently disintegrate, releasing adatoms once again.

The framework for analyzing the K nucleation phase

The classical theory of single-component heterogeneous nucleation was first proposed by Fletcher in 1958.^{16,17} Within the framework of the capillarity approximation, the formation of a K cluster is modelled as a spherical liquid cap with radius r and contact angle θ on a flat surface (Figure 2A; N: nucleus, E: electrolyte, S: substrate). Under the nucleation overpotential η , the Gibbs free energy barrier of the cluster formation (ΔG_{het}) is given by^{18–20}

$$\Delta G_{het} = -\frac{4\pi}{3}r^3F\rho_m\eta f(\theta) + 4\pi r^2\gamma_{NE}f(\theta) \quad (\text{Equation 1})$$

where F is the Faraday constant, ρ_m is the molar density of K atoms in the cluster, and γ_{NE} denotes the nucleus (N)/electrolyte (E) interfacial energy. The shape factor $f(\theta)$ is defined as

$$f(\theta) = \frac{(2+\cos\theta)(1-\cos\theta)^2}{4} \quad (\text{Equation 2})$$

The function $f(\theta)$ increases monotonously from 0 at $\theta = 0$ to 1 at $\theta = \pi$. Under nonwetting conditions ($\theta = \pi$), the cluster adopts a spherical shape, and the process aligns with homogeneous nucleation on metallic K. Consequently, the barrier of heterogeneous nucleation ($0 < \theta < \pi$) is always smaller than homogeneous nucleation barrier (ΔG_{hom}) under identical temperature and entropy conditions.²¹

The nucleation theory, having been extensively utilized in electroplating processes within aqueous solutions, has demonstrated its efficacy in elucidating the nucleation phenomena occurring in non-aqueous alkali metal batteries.^{22–24} Of particular interest, the recent *in situ* electron microscopy observations have brought to light the formation of spherical-cap nuclei in Li electrodeposition.²⁵ It is plausible to anticipate a similar spherical-cap nucleation process for K as well. Consequently, we can confidently employ the nucleation theory as a robust analytical framework to study the nucleation and growth dynamics

within PMBs, which is expected to yield valuable insights into optimizing the electrodeposition processes for K metal anodes.

The contact angle factor

Equations 1 and 2 reveal that a smaller θ corresponds to a lower ΔG_{het} . Furthermore, as θ increases, the growth mechanism transitions sequentially from the Frank-van der Merwe mechanism to the Stranski-Krastanov mechanism and finally to the Volmer-Weber mechanism (Figure 2B). While the precise critical values of θ that trigger these transitions remain incompletely understood, the overall trend has been empirically validated.¹³ Consequently, enhancing the wetting properties of the substrate by decreasing the contact angle of K metal has become a key strategy for realizing dendrite-free K deposition. Surface chemistry modifications, such as surface coatings,¹³ functional groups,²⁶ and surface defects,²⁷ along with structural engineering strategies, including 3D architectures,¹⁴ crystallographic orientation,²⁸ and surface roughness,²⁹ are effective approaches for designing potassiophilic substrates with low contact angles. Mitlin's group altered K wettability by using three substrates: a wettable O-functionalized carbon cloth, a non-wettable non-functionalized carbon cloth, and a Cu foil.³⁰ Their findings highlight the crucial role of substrate wettability in governing K nucleation, deposition morphology, and dendrite formation, as evidenced by improved potassiophilicity from a smaller contact angle with molten K. Potassiphobic substrates tend to produce spongy deposits with dendrites and nanopores, whereas potassiophilic substrates facilitate dense, pore-free deposition. Their meso-scale computational model suggests that strong K-substrate adhesion, comparable to or exceeding K-K cohesion, enhances K nucleus coverage, decreases deposit contact angle, and promotes uniform growth. This aligns with classical electrodeposition theory, where the adhesion-to-cohesion ratio governs the transition among the Frank-van der Merwe, Stranski-Krastanov, and Volmer-Weber growth modes.¹⁵

The surface energy factor

Although contact angle is theoretically a suitable parameter for evaluating potassiophilicity and wettability, contact angle measurements for molten alkali metals are often considered

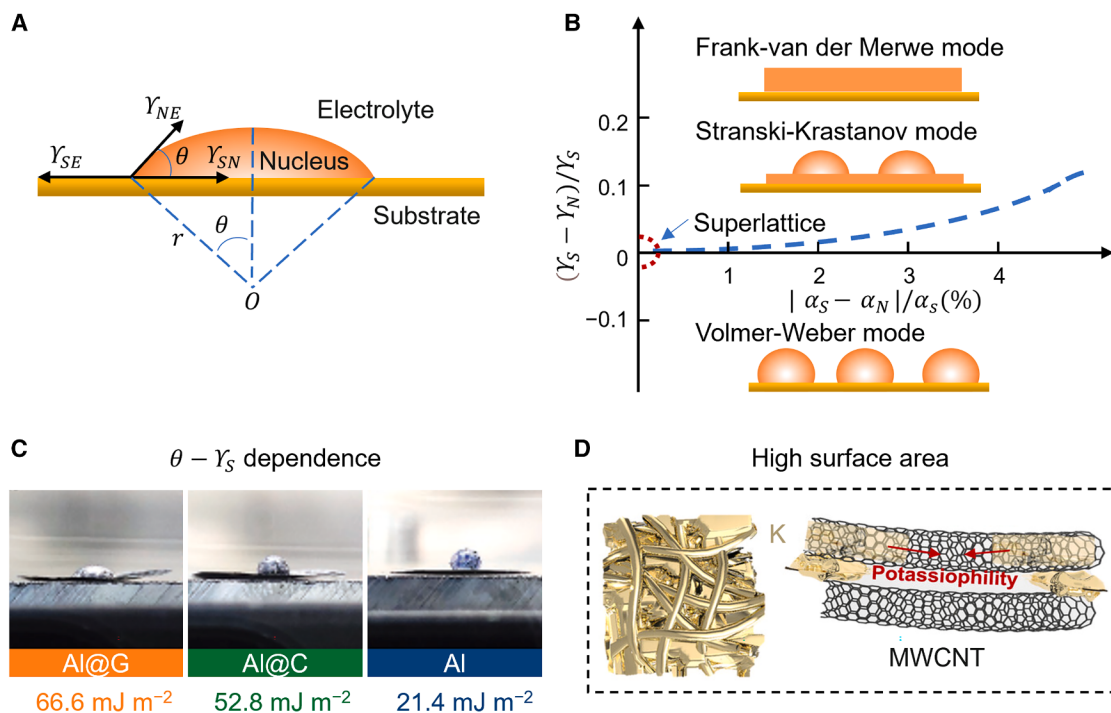


Figure 2. Thermodynamic principles of nucleation and growth

(A) Schematic of the heterogeneous nucleation model, depicting the electrolyte (E), K nucleus (N), and planar substrate (S) as distinct phases. Here, θ denotes the contact angle, and γ represents the surface or interfacial energy of the respective phases.

(B) Stability regions of growth modes, mapped in terms of the surface energy difference between the growing film and the substrate ($(\gamma_S - \gamma_N)/\gamma_S$, vertical axis) and the lattice misfit ($|\alpha_S - \alpha_N|/\alpha_S$, horizontal axis). Here, α represents the lattice constant. The blue dashed line in the graph delineates the transition between the Stranski-Krastanov and Volmer-Weber modes for film growth. Adapted from Wang et al.¹²

(C) Experimental validation of the $\theta - \gamma_S$ dependence, as observed in the wetting behavior of molten K on diverse substrates with varying surface energies. Adapted from Zhao et al.¹³

(D) Diagram depicting the formation of the K/MWCNT composite anode and infiltration of K into MWCNTs. Adapted from Wang et al.¹⁴

qualitative due to inconsistencies in experimental results. The inconsistencies primarily stem from substrate passivation layers, surface roughness, topographical discontinuities, and surface inorganics on the molten alkali metals (mainly oxides and carbonates).³¹ These factors, along with the temperature sensitivity of molten metal contact angles due to temperature-dependent viscosity variations, undermine their quantitative reliability, despite their widespread use in revealing general wetting trends.³² Moreover, in a practical battery system, alkali metal nucleation occurs at room temperature with solid rather than liquid nuclei, leading to a contact angle that differs significantly from those of molten alkali metals.³³ Consequently, substrate surface energy assessment has emerged as a more practical alternative for evaluating potassiophilicity and wettability without relying on molten metal measurements. Surface energy is related to contact angle by the Young-Dupré equation:

$$\cos\theta = \frac{\gamma_{SE} - \gamma_{SN}}{\gamma_{NE}} \quad (\text{Equation 3})$$

where γ_{SE} and γ_{SN} represent the substrate (S)/electrolyte (E) and substrate (S)/nucleus (N) interfacial energies, respectively.

Assuming electrolytes have a negligible effect on substrates' surface energy, a substrate with a high surface energy γ_S should exhibit a low contact angle. The surface energy of air-stable substrates can be readily measured using the Owens method.^{34,35} This approach involves measuring the contact angles of two liquids with known surface energies—one highly polar (e.g., water) and one nonpolar (e.g., ethylene glycol or hexadecane)—to capture diverse solid-liquid interactions. As shown in Figure 2C, Sun's group realized a potassiophilic surface of defect-rich graphene layers (130–150 nm thickness) on commercial Al foils (Al@G), with a high surface energy of 66.6 mJ m⁻², surpassing carbon-coated Al foils (Al@C, 52.8 mJ m⁻²) and bare Al foils (21.4 mJ m⁻²).¹³ The increasing substrate surface energy from bare Al to Al@C and further to Al@G correlates with the decrease in molten K contact angles, indicating strong potassiophilicity and a low ΔG_{het} for Al@G, as described by Equations 1 and 2. This enhanced wettability, attributed to high surface energy of Al@G (Equation 3), facilitates smooth K deposition following the Frank-van der Merwe growth mode (Figure 2B) and extends plating/stripping cycle stability to 1,000 h at 0.5 mA cm⁻². An even higher surface energy of 218.5 mJ m⁻², 5.15 times greater than porous Al (42.4 mJ m⁻²), was achieved by the same group via using nitrogen-doped graphene as the modification layer on

porous Al, further improving potassiphilicity and promoting uniform K growth.³⁶

For substrate materials with insufficient surface energy, potassiphilicity can be improved by increasing the available surface area for K nucleation, which is one of the key reasons for employing 3D host architectures.³⁷ For instance, although multiwalled carbon nanotubes (MWCNTs) have a lower surface energy (28.0 mJ m^{-2}) compared with porous Al (42.4 mJ m^{-2}), the high specific surface area ($92.2 \text{ m}^2 \text{ g}^{-1}$) of MWCNTs compensates for this limitation (Figure 2D).^{14,36,38} Additionally, other factors contribute to their effectiveness in stabilizing K electrodeposition. MWCNTs can undergo potassiation to form potassium carbide (KC_8), which significantly improves potassiphilicity by decreasing the contact angle of molten K.^{39,40} Moreover, the MWCNT matrix provides abundant K nucleation sites, accommodates volume changes, and offers high thermal stability, excellent processability, and flexibility.

It is important to note that increasing the available surface area does not necessarily require creating a rough surface, as excessive roughness can exacerbate K dendrite growth. A recent study from Lu's group demonstrated this by coating a fluorine-doped graphene oxide (F-GO) layer onto K metal foil.⁴¹ This innovative coating smoothens the substrate surface while generating a uniform electric field that mitigates the "tip effect"—a phenomenon where K ions accumulate at surface protrusions, causing uneven deposition and dendrite formation. Concurrently, the porous structure of the F-GO layer increases the available surface area within its framework for K deposition. Thus, careful design of substrate surface structures is essential for realizing high surface energy without an overly rough surface.

Simplifying K nucleation with the binding energy factor

Building on the wettability principles established in [The framework for analyzing the K nucleation phase](#), we now examine binding energy as a critical atomic-scale descriptor of K-substrate interactions. Nucleation is inherently site-specific and can be conceptually simplified as a series of point-to-point interactions, emphasizing the role of localized adsorption sites (Figure 3A). Binding energy quantifies the adsorption strength between K ions/atoms/clusters and specific substrate sites, making it particularly effective for analyzing materials with heterogeneous active sites such as heteroatoms, nanoparticles, or alloy phases that differ significantly from their surroundings. While surface energy and contact angle offer a macroscopic framework for nucleation thermodynamics (Equations 1–3), binding energy provides complementary atomic-scale insights into site-specific adsorption processes relevant to the early stages of nucleation, including adsorption and clustering. These active sites facilitate K-ion reduction to adatoms, lower the nucleation overpotential, and promote uniform nucleation. Effectively, binding energy also influences whether K adatoms/clusters remain anchored or diffuse across the substrate surface.

In this context, first-principles calculations serve as a powerful tool for simulating the binding energy of K ions/atoms/clusters on anode substrates. While binding energy broadly encompasses both strong interactions, such as covalent, ionic, and metallic bonds, and weaker forces, including van der Waals and hydrogen bonding, adsorption energy specifically refers to

surface interactions governed by physisorption or chemisorption. In many cases, adsorption energy and binding energy are used interchangeably, particularly when (1) a strong and stable interaction between K and the anode substrate results in a configuration with significantly lower energy than that of the non-interacting components; (2) the system consists of small entities, such as individual atoms or small molecules, where the distinction between adsorption energy and binding energy is negligible; or (3) adsorption leads to the formation of new bonds or significant modifications to existing bonds, including covalent, ionic, or metallic interactions. For clarity and consistency, the term "binding energy" will be used throughout this discussion.

Increasing binding energy via heteroatom doping

Porous carbon hosts with heteroatom doping strongly adsorb K atoms, enabling efficient charge transfer and ensuring uniform nucleation and growth. Using first-principles calculations, Zhang's group explored the effects of diverse heteroatom doping (B, N, O, F, P, S, Cl, Br, and I) in carbon materials on their potassiphilicity (Figure 3B).⁴² Their results reveal that strong adsorption arises from significant local dipoles between the doping atom and its adjacent atom, along with a critical charge transfer (Bader charge) of at least 0.89 e^- from the K atom to the dopant. Based on this, the authors identified carboxylic groups ($-\text{COOH}$) and B–2C–O-type boron as optimal configurations for mono- and co-doping scenarios. The theoretical predictions have been extensively validated by experimental studies using O-containing groups in doped carbon substrates.^{26,39,44–47} For instance, oxygen-containing functionalized porous carbon microbelts (OPCMs), synthesized via chemical exfoliation and enzyme-assisted synergy, enable K-OPCM composite anodes to achieve lower overpotential ($\sim 40 \text{ mV}$) and extended cycle life (over 800 h) at 1 mA cm^{-2} , compared with bare K anodes in symmetric cells.⁴⁴ In addition, other heteroatom doping strategies, such as N doping,⁴⁸ P doping,⁴⁹ N/O co-doping,⁵⁰ N/O/S co-doping,⁵¹ and amine functional groups,⁵² have also shown enhancement in K electrodeposition. For example, P-doped porous carbon nanofibers infused with K, when paired with perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) cathodes, exhibit exceptional cycling performance, achieving an 85% capacity retention after 1,000 cycles at a rate of 20 C .⁴⁹

Increasing binding energy via inorganic nanoparticles

Beyond heteroatom doping, incorporating inorganic nanoparticles into a carbon host or applying an inorganic layer to a current collector (e.g., Cu and Al) has also shown significant promise. Inorganic materials adsorb K ions or atoms primarily through electrostatic interactions and chemical bonding (chemisorption). For instance, uniformly dispersing CoWO_4 nanoparticles within a honeycomb porous carbon matrix significantly enhances its potassiphilicity, increasing the binding energy of K ions on the porous carbon matrix by 3.88 times, from -0.57 eV to -2.21 eV .⁵³

Several key factors must be considered when selecting inorganic nanoparticles to enhance the binding energy of the substrate or host toward K and thus improve K electrodeposition. Given the complexity of these requirements, it is challenging to find a single material that excels in all aspects; however, it is essential to excel in as many aspects as possible.

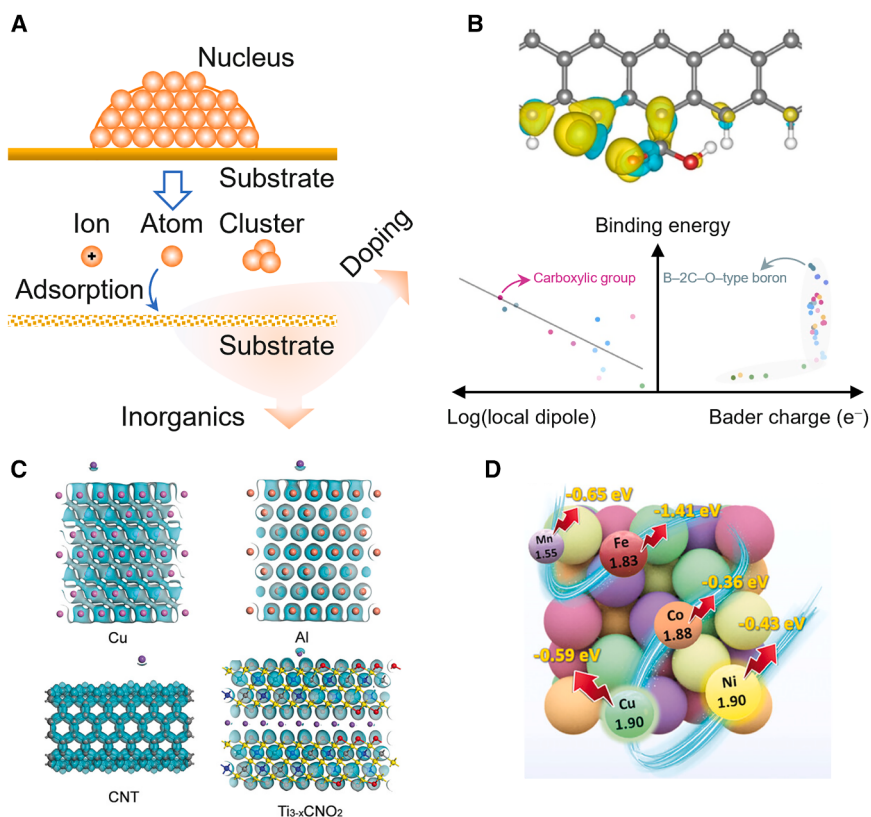


Figure 3. Principles of adsorption during nucleation

(A) Illustration of a simplified nucleation model, showcasing the adsorption of an individual ion/atom/cluster onto the substrate surface.

(B and C) To enhance adsorption efficiency, two principal methodologies are implemented: heteroatom doping (B) and the deployment of inorganic materials (C). (B) Upper panel: a computational model based on first principles and the accompanying differential charge density for K adsorption on an oxygen-doped carbon surface featuring a carboxylic functional group. Distinct atoms are represented by varied colors: oxygen (red), hydrogen (white), and carbon (gray). Lower panel: the binding energy in correlation with local dipole and charge transfer across different doping configurations. *Reproduced from Chen et al.*⁴² (C) DFT constructs and the resultant deformation charge density for K atoms adsorbed onto Cu, Al, CNT, and $Ti_{3-x}CNO_2$ substrates. *Reproduced from Tang et al.*²⁷

(D) Comparative electronegativity values for constituent elements within an HEA. *Adapted from Chang et al.*⁴³

- (1) Compatibility: inorganic nanoparticles should be chemically compatible with PMBs, maintaining stability under electrochemical conditions and negative potentials without significant degradation.
- (2) Structural stability: materials should retain their structural integrity during cycling, which, in some cases, directly correlates with their electrochemical stability (1).
- (3) Conductivity: highly conductive materials, including metals,^{54–58} bimetallics,^{59–62} and some compounds (e.g., MoC^{63}), are beneficial to ensure efficient charge transfer and ion diffusion.
- (4) High surface area and porosity: materials such as metal-organic frameworks⁶⁴ and transition metal oxides^{65,66} can offer abundant active sites for K adsorption, while their porous structures facilitate efficient K-ion diffusion.
- (5) Electrochemical activity: redox-active materials can improve K-ion adsorption and desorption during charge/discharge cycles. Candidate materials can be drawn from electrode materials used in PIBs, such as transition metal oxides and sulfides.⁶⁷

Inorganic materials with rich surface chemistries further enhance K adsorption. MXene, with its tunable composition and diverse chemical properties, has shown great potential for improving K binding energy. A defect-rich, nitrogen-containing MXene synthesized by removing Al atoms from the Ti_3AlCN precursor, a process that facilitates carbon substitution by nitrogen within the MXene layers, exhibits a notable K binding energy

of -1.91 eV, which further increases to -2.27 eV with the introduction of a Ti vacancy.²⁷ As shown in Figure 3C, these values significantly surpass the binding energies of Cu (-0.13 eV), Al (-0.51 eV), and CNT (-0.84 eV). The enhanced binding energy supports K nucleation, as evidenced by a substantially lower nucleation overpotential of ~ 6 mV, compared with a control value exceeding 33 mV.

Intriguingly, high-entropy alloys (HEAs), composed of five or more metallic elements in near-equal or equimolar ratios, enhance K binding energy and increase the density of active nucleation sites through local electron redistribution driven by electronegativity differences (Figure 3D).^{43,68} Unlike simple alloys, elemental segregation and aggregation in HEAs create alternating regions of electron accumulation and depletion within the surface layers.⁶⁹ Chemical redistribution in the surface layer, driven by the segregation of alloying atoms, can result in localized variations in surface energy at the atomic or short-range order scale. This has been demonstrated by density functional theory (DFT) calculations on equimolar face-centered cubic (FCC) $AgAuCuPdPt$.⁷⁰ The (111) surface of $AgAuCuPdPt$, for instance, exhibits significant segregation, with enrichment of Au and Ag and depletion of Cu, Pd, and Pt in the surface layer, resulting in a surface energy distribution that is considerably broader than that of the bulk (0.0813 eV versus 0.0317 eV per square root number of atoms). Localized high surface energies correlate with increased binding energies, thereby enhancing potassio-philicity.⁷¹ Additionally, lattice distortion in HEAs raises their potential energy, further lowering the energy barrier of

adsorption.⁷² HEAs feature an inherently complex compositional space, arising from the vast array of possible element combinations and their varying proportions. This complexity necessitates the use of high-throughput experimentation and data-driven strategies, which are well-suited for systematically tuning HEA compositions and exploring their properties in the context of K anodes.^{73,74}

The use of binding energy to predict nucleation in K electrodeposition is a theoretical approach based on the energy released for K ions or atoms to adsorb onto the anode surface. However, this method has limitations. Unlike heterogeneous nucleation theory, which quantifies the nucleation energy barrier through thermodynamic free energy changes, the empirical correlation between high ion/atom/cluster binding energy at nucleation sites and uniform nucleation lacks a comprehensive theoretical framework. Specifically, although high binding energy has been experimentally related to low nucleation overpotential, a quantitative correlation between binding energy and the nucleation energy barrier remains undefined. By contrast, heterogeneous nucleation theory provides a well-established quantitative framework, linking the nucleation energy barrier to surface and interfacial energies (i.e., nucleus-substrate wettability) and electrochemical driving forces such as overpotential and current density.^{18,23,75} Moreover, while nucleation typically initiates at the nanoscale to sub-micron scale, subsequent growth and morphological evolution extend to the micron scale. Binding energy calculations at the atomic scale may fail to capture this multiscale behavior, particularly as the binding energy per atom often varies with cluster sizes.⁷⁶ Integrating DFT with multiscale modeling frameworks is essential to bridge this gap, which will be discussed in the prospects.

Combining binding energy and interfacial energy

In [The framework for analyzing the K nucleation phase](#), the interplay between contact angle and surface energy elucidates the K nucleation mechanism, conceptualizing the K cluster as a spherical droplet cap. [Simplifying K nucleation with the binding energy factor](#) delves into how binding energy streamlines nucleation into a sequence of localized interactions. Both models assume that the substrate's chemical properties remain predominantly unaltered, thereby preserving the K/substrate interface. If the interface is disrupted by atomic diffusion or chemical reactions, leading to the formation of a new interface for subsequent nucleation, a combined analysis of binding and interfacial energies provides valuable insights into this complex process.

This combined analysis is particularly evident in K-alloying materials, where alloying serves as a strategy to anchor K atoms to alloying seeds, optimizing binding energy to promote nucleation.⁷⁷ However, the nucleation process remains uncertain, as binding energy primarily reflects the strength of alloying reactions rather than fully capturing K-substrate nucleation interactions; therefore, interfacial energy should be taken into consideration.

Due to alloying reactions, the K metal/alloy seed interface exhibits negative interfacial energy, leading to the formation of an intermediate alloy layer that serves as a distinct substrate for K nucleation ([Figure 4A](#)).⁷⁹ The transition from alloying to nucleation occurs when the interfacial energy (γ_{IN}) between the intermediate layer and K approaches zero. As per [Equation 3](#), this

condition minimizes the contact angle, thereby enhancing potassiumophilicity and lowering the nucleation energy barrier, which is favorable for stable and efficient plating/stripping cycles. The synergy between binding energy and interfacial energy is critical: strong binding energy ensures selective K deposition on alloying seeds, while decreased interfacial energy promotes a more wettable interface.

Xie's group fabricated a K host consisting of monodisperse amorphous Zn clusters embedded in hierarchically porous nitrogen-doped carbon (NC) fibers.⁷⁷ As shown in [Figure 4B](#), DFT calculations reveal a binding energy of 2.05 eV for a K atom interacting with NC. The binding energy increases to 2.94 eV upon the introduction of a Zn cluster, demonstrating strong binding of K atoms to Zn clusters as alloying seeds. Similarly, Lu's group developed a flexible, self-supporting K host by incorporating a Bi composite into a nitrogen-doped reduced graphene oxide film ([Figure 4C](#)).⁷⁸ The spontaneous alloying reaction between Bi and K is driven by the strong K-Bi binding energy, which facilitates selective K deposition on Bi seeds. Simultaneously, an intermediate K-Bi alloy layer forms, decreasing interfacial energy with K and creating an ideal substrate for K nucleation with an impressively low nucleation overpotential of ~5 mV. This synergistic mechanism effectively suppresses dendrite growth, ensuring a stable and uniform electrodeposition process. As shown in [Figure 4D](#), evenly distributed alloying seeds afford well-defined nucleation sites, each with a lowered nucleation energy barrier, thereby effectively directing K nucleation and alleviating the uneven deposition commonly encountered in PMBs.

Alloying seeds can be introduced through direct alloying reactions with metals such as Sn,⁸⁰ Sb,⁸¹ Bi,^{82,83} Zn,^{77,84} and Hg,⁸⁵ or indirect alloying following conversion reactions with compounds like SnS₂,⁸⁶ SnO₂,^{87–89} Sb₂O₃,⁹⁰ ZnO,^{91,92} and GeO₂.⁹³ Prior to nucleation, the formation of an intermediate alloy layer with high K affinity acts as a buffer, facilitating efficient nucleation. However, this mechanism becomes uncertain for alloy seeds with high K solubility, such as Bi, Sb, and Sn. These elements form alloys like K₃Bi,⁹⁴ K₃Sb,⁹⁵ K₂Sn₅, and K₄Sn₂₃^{96,97} and are widely used as alloying-type anodes in PIBs. In such systems, intense alloying reactions may outweigh K electrodeposition, necessitating further in-depth investigation.

THE IMPACT OF THE SEI ON K NUCLEATION AND GROWTH

The SEI is nonnegligible when investigating K electrodeposition, creating new interfaces of K/SEI and substrate/SEI besides the existing substrate/K interface. K-SEI forms more readily than Li- and Na-SEIs due to the high reducing ability of K. Contact with an electrolyte prompts the immediate formation of a chemically induced SEI on K. As PMBs start cycling, additional SEI layers are deposited, resulting from the electrochemical breakdown of the electrolyte under operating conditions. As shown in [Figure 5D](#), SEI is a nanometer-thin layer composed of both organic and inorganic components. It acts as a critical physical barrier between the anode and the electrolyte, effectively preventing electron flow while enabling ion transport. Such dual functionality not only shields the battery from detrimental electrochemical reactions but also inhibits dendrite formation. It is

noteworthy that electron tunneling can only occur if the SEI thickness is less than 10 Å, which means the SEI discussed here is effectively electron-insulating.¹⁰⁰ Given the essential role of the SEI as both a physical barrier and an ion transport medium, the mechanical strength and ionic conductivity of the SEI are pivotal in determining its overall effectiveness. Furthermore, the mechanical properties and ion conduction capabilities of the SEI layer are intricately linked to the nucleation behavior of K metal. Consequently, elucidating the relationships of composition-mechanical strength and composition-ionic conductivity is crucial for uncovering the underlying mechanisms that govern K electrodeposition performance.

Mechanical strength of the SEI

K electrodeposition subjects the SEI to mechanical pressure from the expanding K metal around the deposition sites. According to heterogeneous nucleation theory, the presence of the SEI creates new interfaces, i.e., the substrate/SEI and nucleus/SEI interfaces shown in Figure 5A instead of the substrate/electrolyte and nucleus/electrolyte interfaces shown in Figure 2A. The Young-Dupré equation is modified as follows:

$$\cos\theta = \frac{\gamma_{SS'} - \gamma_{SN}}{\gamma_{NS'}} \quad (\text{Equation 4})$$

where S' represents the SEI layer, and $\gamma_{SS'}$, γ_{SN} , and $\gamma_{NS'}$ denote the substrate/SEI, substrate/nucleus, and nucleus/SEI interface energies, respectively.

Assuming K deforms due to a pressure difference (ΔP) across the nucleus/SEI interface, for a spherical-cap nucleus with orthogonal radii of surface curvature R_1 and R_2 , ΔP is given by the Laplace pressure:¹⁰¹

$$\Delta P = \gamma_{NS'}(1/R_1 + 1/R_2) \quad (\text{Equation 5})$$

For a given nucleus, Equations 4 and 5 indicate that a lower nucleus/SEI interface energy lessens the pressure difference and contact angle, indicating stronger interfacial adhesion, which stabilizes the interface. Importantly, the mechanical strength of the SEI is critical in counteracting stress, particularly during the nucleation phase when the nucleus size is small. A mechanically robust SEI resists fracture, ensuring the stability of the nucleus/SEI interface and significantly improving overall cell performance of PMBs.

Kang's group investigated how the distinct mechanical properties of SEIs on Li and K anodes influence their growth mechanisms.⁹⁸ In carbonate electrolytes, the Li-SEI, rich in Li_2O and lithium ethylene dicarbonates ($(\text{CH}_2\text{OCO}_2\text{Li})_2$), exhibited enhanced strength and flexibility,^{102,103} whereas the K-SEI, deficient in K_2O and dominated by alkyl carbonates ($\text{CH}_2\text{ROCO}_2\text{K}$), was more fragile. As shown in Figure 5B, the atomic force microscopy (AFM) nanoindentation force-displacement curve for Li reveals sequential elastic and plastic deformation of the SEI, followed by elastic deformation of underlying Li as displacement decreases, with a force plateau at ~ 1 μN indicating durable plastic deformation. By contrast, a force dip at ~ 100 nN for K (Figure 5C) signifies SEI fracture under stress, highlighting the low mechanical integrity of the K-SEI. This fragility leads to cracking and fragmentation during deposition, driving distinct

K growth behavior. The robust Li-SEI directs Li growth from the root where the SEI is thinnest, forming whisker-like, anisotropic dendrites ("needles"). By contrast, the weak K-SEI fractures under local stress, exposing fresh surfaces for nucleation and resulting in isotropic, granular "forest-like" K dendrites (Figures 5B and 5C). To quantitatively evaluate the mechanical strength of SEI, Young's modulus (E) and elastic strain limit (ϵ_Y) have been used to show the dependence of mechanical strength on SEI compositions.^{104,105} As the K salt (bis(fluorosulfonyl)imide (KFSI)) concentration increased from 0.25 to 2 M, E increased while ϵ_Y declined, reflecting an increase in the inorganic components in the SEI (Figure 5D). As a result, a balance was reached between the two at 0.5 M to obtain the most resilient SEI, i.e., the optimal SEI strength, as an imbalance (e.g., low E at 0.25 M or low ϵ_Y at 2 M) can cause dendritic K growth and degrade cell performance. This is consistent with the formation of a robust Li-SEI comprising a mixed inorganic-rich and organic-rich double layer, in contrast to a less stable single inorganic-rich layer.¹⁰⁶

Ionic conductivity of the SEI

The ionic conductivity of SEIs is typically several orders of magnitude lower than that of liquid electrolytes (e.g., 10^{-12} to 10^{-4} S cm^{-1} for SEIs versus 10^{-3} to 10^{-2} S cm^{-1} for liquid electrolytes).^{107,108} This makes ion transport through SEI the rate-limiting step in the overall process, which determines the exchange current density of the cell, highlighting the critical importance of the ionic conductivity of SEI.

Experimental studies consistently show that SEI resistance depends more on its composition than thickness, with higher inorganic content enhancing ionic conductivity.¹⁰⁹ For instance, Sun's group demonstrated the formation of an inorganic-rich SEI using a N-doped graphene-coated porous Al current collector (NG@P-Al).³⁶ The electronegativity difference between the N-doped carbon and the Al substrate reduces the electron density on Al, prioritizing electron transfer to the electrolyte salt over the solvent and thus promoting the formation of an inorganic-rich SEI. Such SEI layers exhibited significantly high ionic conductivity and low activation energy, a finding corroborated by other studies.¹⁰⁴

Inorganic components in SEI are complex and depend on the electrolyte, while KF, K_2O , and K_2CO_3 are the most commonly observed, with K_2SO_4 appearing in S-containing electrolytes.^{36,110,111} Unfortunately, the ionic conductivities of these compounds in PMBs remain uncharacterized. Bond-valence energy landscape (BVEL) calculations reveal that the K diffusion energy barrier in KF is as high as 1.44 eV (Figure 5E), indicating that KF is highly ionically insulating and that ion migration through it is kinetically unfavorable,¹¹² evidenced by the increased charge transfer resistance of fluoroethylene carbonate (FEC)-derived KF-rich SEI.^{113,114} As a result of the high K diffusion energy barrier in KF, K-ion conduction likely occurs through other, more conductive inorganic components or grain boundaries in the SEI, which is verified in lithium metal batteries, yet a hypothesis that requires further computational and experimental validation for PMBs.

To enhance the ionic conductivity of the SEI, enriching it with ion-conductive inorganic compounds has proven effective. A positive attribute is observed in K_2S and K_2Se , as both

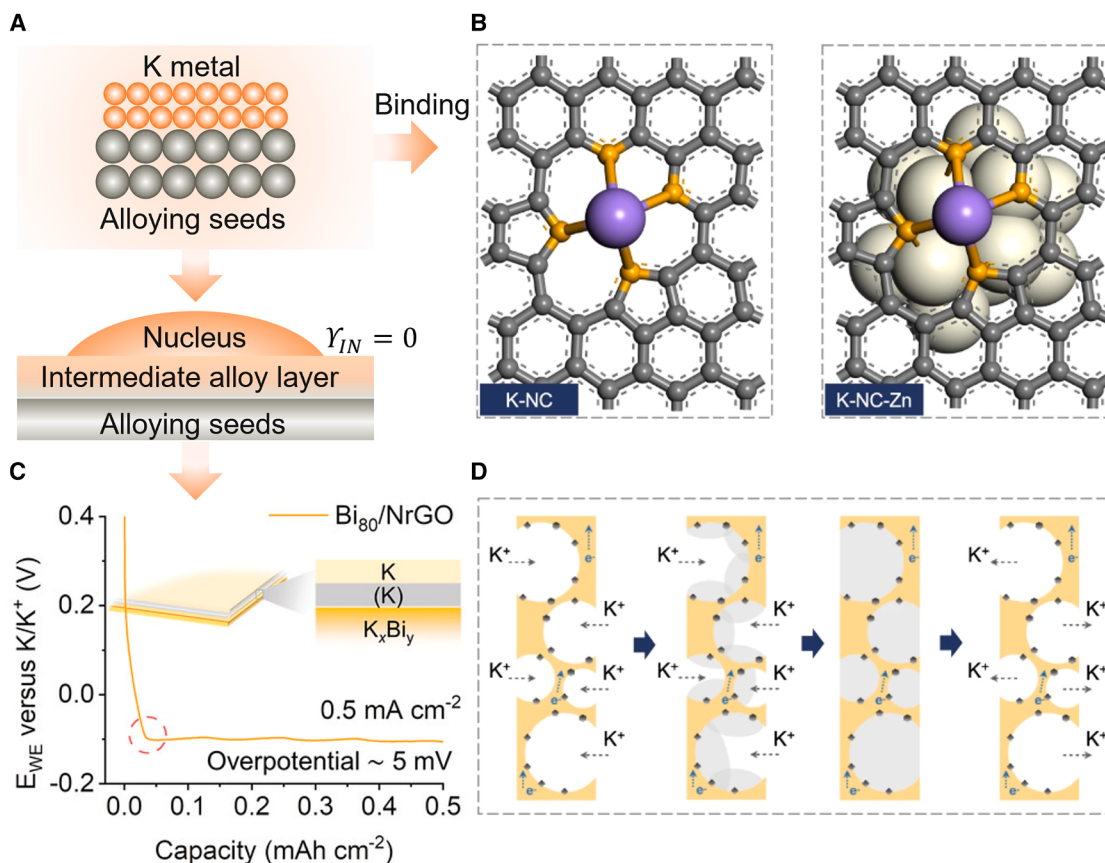


Figure 4. Integrating binding and interfacial energies in K nucleation via alloying seeds

(A) Schematic illustration of the K metal/alloying seed interface, which is conceptualized as the binding of a K atom to the seed or nucleation on an intermediate alloy layer that eliminates interfacial energy (γ_{IN}).

(B) DFT models depicting a K atom binding to distinct substrates. Adapted from Li et al.⁷⁷

(C) Voltage profile for K plating on a Bi_{80}/N -doped rGO substrate at a current density of 0.5 mA cm^{-2} , with the red dashed circle highlighting the minimal overpotential for K plating. The inset illustrates the role of the alloy buffer layer between Bi and K in lowering the nucleation barrier. Adapted from Feng et al.⁷⁸

(D) Diagram showing selective K plating and stripping on alloying seeds (dark dots) that are uniformly distributed within a porous carbon matrix (yellow structure). Adapted from Li et al.⁷⁷

compounds demonstrate rapid K-ion migration along the [100] and [110] crystallographic directions.^{112,115} Their integration within the SEI facilitates K-ion diffusion for dendrite suppression. Moreover, Yu's group treated K metal with red phosphorus powders to form K_xP_y , which reduced the activation energy for K-ion conduction in the SEI from 70.7 kJ mol^{-1} to 55.7 kJ mol^{-1} and increased the exchange current density from 1.14×10^{-5} to $3.52 \times 10^{-5} \text{ mA cm}^{-2}$.¹¹⁶ The enhanced ionic conductivity of the SEI decreases voltage hysteresis and significantly extends the cycle life of symmetric K||K cells from 55 to 550 h at 0.5 mA cm^{-2} . They achieved similar results using tellurium (Te) powders to form K_2Te . *Ab initio* molecular dynamics (AIMD) simulated trajectories of a K ion in K_2Te reveal the [100] direction as the most favorable pathway for K-ion migration (Figure 5F).⁹⁹

The SEI is dynamic rather than static. Recent *operando* AFM and X-ray photoelectron spectroscopy (XPS) studies have elucidated the morphological and compositional evolution of the Li-SEI. *Operando* AFM results revealed a two-stage SEI growth on Cu foil: a reaction-limited formation of a dense, passivating

primary layer driven by ion-coupled electron transfer, and a subsequent diffusion-limited growth of a porous secondary layer.¹¹⁷ *Operando* XPS, performed under near-ambient pressure ($\sim 0.25 \text{ mbar}$), confirmed the formation of Li_2CO_3 , lithium alkylcarbonates, and LiF, with binding energy shifts relative to potential providing indirect spatial information.¹¹⁸ Currently, the dynamic evolution of the K-SEI remains largely unexplored, particularly how its structural and compositional features influence mechanical strength and ionic conductivity, which are key factors affecting K electrodeposition. The SEI also undergoes repeated rupture and reformation during plating/stripping.^{119,120} A deeper understanding of these processes, along with the role of individual SEI components, is vital for rational interfacial design and the development of stable PMBs.

SUMMARY AND PROSPECTS

K dendrite growth remains a critical and unresolved challenge for K metal anodes, necessitating stable and long-term

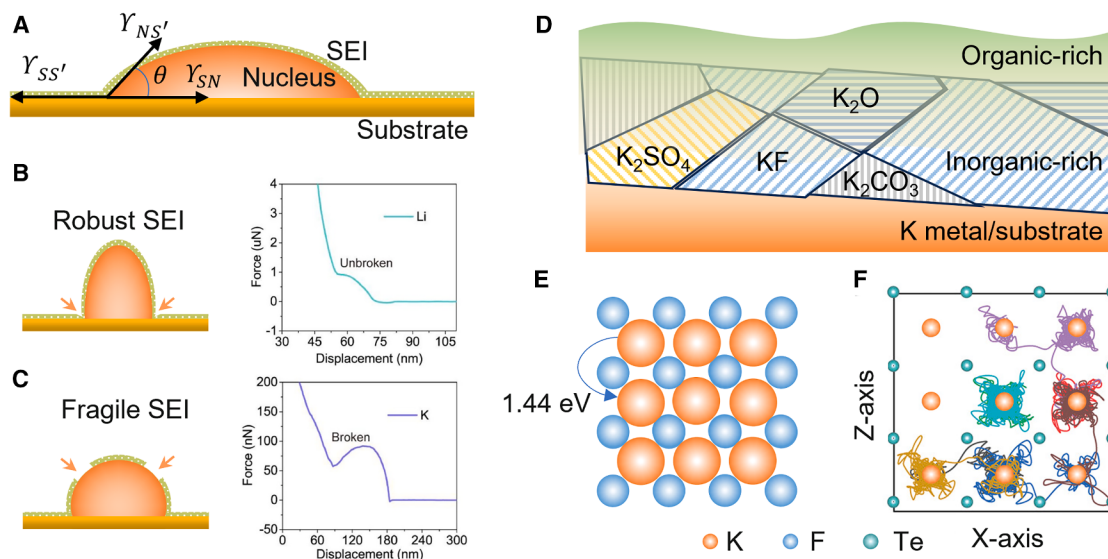


Figure 5. The impact of the SEI on K nucleation dynamics

(A) The heterogeneous nucleation model accounting for the presence of the SEI layer.

(B and C) Left: schematic depictions of the root growth mode for Li deposition and the surface growth mechanism for K deposition. Right: representative force curves obtained from AFM nanoindentation of Li and K metal foils, both covered by an SEI layer. *Reproduced from Hu et al.*⁹⁸

(D) Structural schematic of the SEI formed on K metal or its substrate, featuring an inorganic-rich inner layer and an organic-rich outer layer, with typical crystalline components such as KF, K₂O, K₂CO₃, and K₂SO₄. The inorganic constituents contribute to E , while the organic components affect ϵ_Y .

(E) An atomic-scale view of KF along the {100} plane, revealing a 1.44 eV energy barrier for K-ion migration.

(F) AIMD simulated trajectories of a K ion at 1,600 K within the X-Z plane of K₂Te, with differently colored curves indicating the ion's trajectories at various lattice sites. These trajectories highlight the [100] crystal direction as the predominant migration pathway. *Reproduced from Yang et al.*⁹⁹

electrodeposition to enable practical PMBs. This review presents a theoretical framework for elucidating K nucleation and early-stage growth, grounded in interfacial parameters such as contact angle, surface energy, interfacial energy, and binding energy (Figure 6). By integrating these factors, the framework offers a more nuanced perspective on the thermodynamics and kinetics of K electrodeposition. The influence of SEI is examined in parallel, with emphasis on its mechanical resilience and ionic conductivity. The structural complexity and dynamic evolution of the K-SEI, along with the evolving SEI/K and SEI/substrate interfaces, critically shape nucleation and growth behavior yet require more targeted investigation. Recent experimental advances are also reviewed, underscoring the importance of coupling theoretical insights with materials design to optimize electrodeposition behavior. Together, these insights establish a foundation for predictive, design-oriented strategies to stabilize K metal anodes and accelerate the development of high-performance, sustainable PMBs. To advance this field further, we outline key research directions (Figure 6) aimed at deepening the understanding of K electrodeposition mechanisms and SEI interfacial dynamics.

Work of adhesion as a thermodynamic descriptor for nucleation

Existing nucleation and growth models have been instrumental in elucidating the mechanisms of K electrodeposition. However, their application has primarily been limited to simplified conditions, often neglecting the complexity introduced by SEI-related interfaces. Given the indispensable role of SEI in PMBs, both the

nucleus/SEI and substrate/SEI interfaces must be considered to accurately describe the electrodeposition process.

As discussed in this review, three interfacial energies—the nucleus/SEI, substrate/SEI, and substrate/nucleus interfacial energies—govern the contact angle and nucleation energy barrier. Work of adhesion, W_{adh} , a descriptor that integrates these interfacial energies, should be considered for K electrodeposition. W_{adh} is defined as follows:

$$W_{adh} = \gamma_{NS'} + \gamma_{SS'} - \gamma_{SN} \quad (\text{Equation 6})$$

This expression encapsulates the thermodynamic stability of the nucleus/substrate interface, serving as a comprehensive parameter that accounts for the overall interfacial energies involved in its formation or dissociation. A high W_{adh} corresponds to a more stable interface and a lower contact angle θ , arising from high nucleus/SEI and substrate/SEI interfacial energies and low substrate/nucleus interfacial energy. As a result, W_{adh} can be seen as a robust descriptor of the K nucleation process, providing design guidance for substrates, SEIs, and artificial SEIs. For example, substrates with a high W_{adh} and large accessible surface areas are expected to enhance thermodynamic stability and reduce the nucleation barrier, thereby enabling more uniform K deposition.

Electrolyte engineering to optimize the SEI

Electrolyte engineering is central in tailoring SEI composition to achieve uniform, ionically conductive, and mechanically robust interphases. As salt concentration increases in the electrolyte, ion

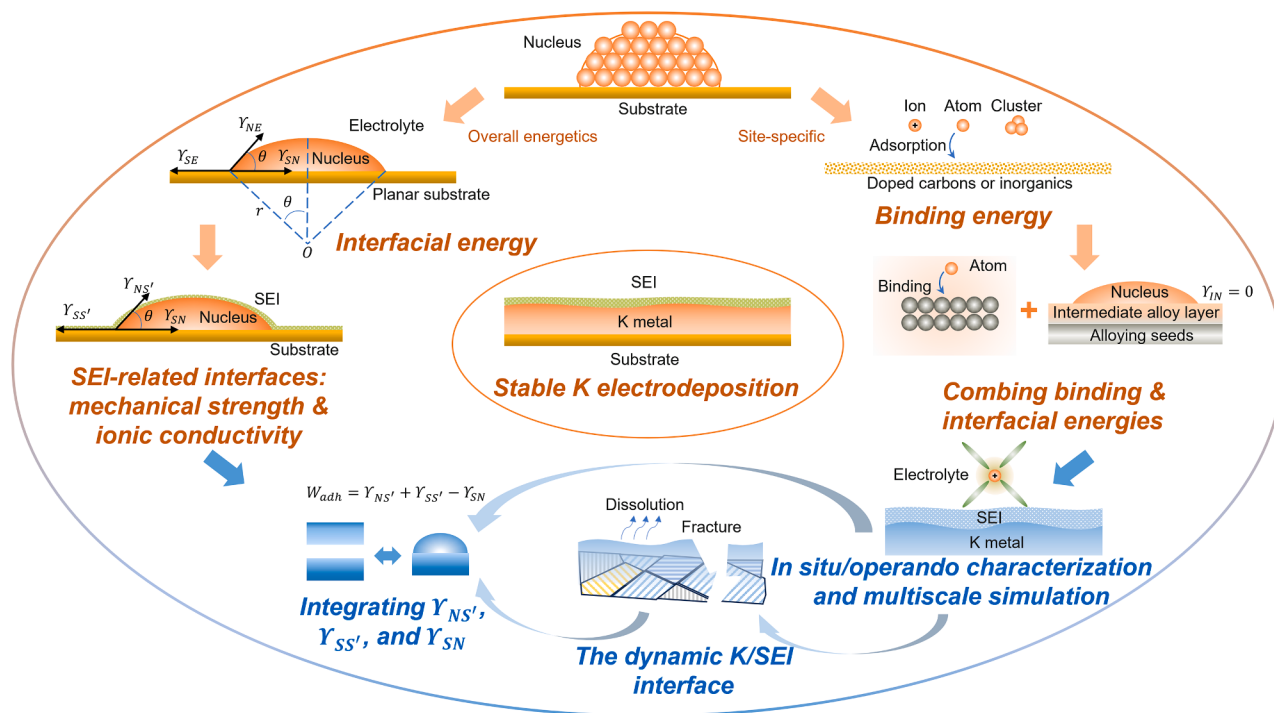


Figure 6. Key factors and future directions for stable K electrodeposition

A schematic overview highlighting the key factors for achieving stable K electrodeposition and future research directions. The crucial factors include energetic parameters such as interfacial energy, binding energy, and their combined effects, along with the mechanical strength and ionic conductivity of the SEI. Future research directions encompass leveraging work of adhesion for optimized substrate design, exploring the dynamic evolution of the K/SEI interface and its impact on K electrodeposition, and gaining deeper experimental insights.

pair structures evolve from solvent-separated ion pairs (SSIPs) to contact ion pairs (CIPs) and ultimately to aggregates (AGGs), depending on the number of cations coordinated with each anion.¹²¹ This progression reduces free solvent availability and reshapes the solvation environment. In high-concentration electrolytes (HCEs), dense ion clustering broadens the electrochemical stability window and favors the formation of inorganic-rich, stable SEI layers. Localized high-concentration electrolytes (LHCEs), which incorporate non-solvating diluents, preserve the beneficial solvation characteristics of HCEs while alleviating drawbacks such as high viscosity, thereby offering a balanced approach to interfacial stability and processability.¹⁰⁰ Further modulation of ion cluster size and packing density can enhance anion reduction kinetics and ion mobility, facilitating the formation of ultrathin, uniform SEI layers and suppressing dendrite growth. Recent studies in lithium electrolytes demonstrate that larger ion AGGs (~3–4 nm) accelerate anion reduction and yield thin, inorganic-rich SEIs,¹²² whereas smaller clusters improve ionic conductivity and foster uniform metal deposition.¹²³ Optimized solvation structures comprising compact anion- Li^+ complexes of intermediate size exhibit high ionic conductivity, low desolvation barriers, and homogeneous inorganic SEI components, underscoring the strong interplay between solvation structure and interfacial stability.¹²⁴ These results may serve as “drop-in” strategies for engineering K electrolytes and SEIs; however, caution is warranted when comparing Li and K systems, as elucidating their fundamental dif-

ferences offers greater insights than merely identifying transferable approaches. Advancing the strategies of electrolyte and SEI optimization requires integrating computational modeling, *in situ/operando* characterization, and multifunctional electrolyte design.¹²⁵ Ultimately, interdisciplinary approaches that unify solvation engineering, interfacial chemistry, and mechanical durability will be essential for achieving high-energy-density, long-cycle-life PMBs.

***In situ/operando* characterization of the anode**

Despite the critical role of the SEI in K electrodeposition, it remains poorly understood due to its compositional and structural complexities, along with its dynamic evolution during cycling—often driven by instability and inhomogeneity.^{126,127} A complete understanding of SEIs and their influences on K electrodeposition requires precise characterization of their structural, chemical, mechanical, and dynamic features. *In situ* and *operando* techniques are particularly valuable, as they enable real-time observation of interfacial processes while avoiding artifacts caused by air exposure, salt precipitation, or the dissolution of semi-soluble layers during post-treatment.¹¹⁷ Although still limited in PMB research, recent studies in Li and Na systems offer important methodological guidance.¹²⁸ A range of advanced *in situ/operando* tools can be employed to probe K electrodeposition, SEI evolution, and interfacial dynamics: (cryo-)electron microscopy for nanostructure and elemental

mapping,¹²⁹ AFM for surface morphology and mechanical properties,¹¹⁷ laser scanning confocal microscopy (LSCM) for dendrite evolution and interfacial dynamics,¹³⁰ X-ray microscopy for 3D defect visualization,¹³¹ XPS for surface chemical state analysis,¹¹⁸ time-of-flight secondary ion mass spectrometry (ToF-SIMS) for molecular-level heterogeneity,¹³² nuclear magnetic resonance (NMR) for ion transport and solvation behavior,¹³³ and depth-sensitive plasmon-enhanced Raman spectroscopy (DS-PERS) for nanostructural and bonding depth profiling.¹³⁴ The integration of these techniques will be essential for elucidating the SEI's chemical composition, mechanical properties, and ionic conductivity and for establishing quantitative relationships among these characteristics and the complex interfacial phenomena that govern K electrodeposition, thereby guiding the design of stable, high-performance K metal anodes.

Multiscale simulation frameworks

Complementing advanced characterization, multiscale simulation frameworks that integrate DFT, molecular dynamics (MD), and phase-field simulations are essential for elucidating the complex processes governing K nucleation and growth. MD simulations offer insights into nanoscale K cluster formation and growth dynamics under realistic electrochemical conditions, while phase-field models incorporating interfacial energy, overpotential, and concentration gradients capture mesoscale morphology evolution, such as dendrite propagation or compact layer formation. These modeling approaches have been successfully applied to Li and Na metal systems to bridge atomic-scale energetics with macroscopic deposition behavior.^{135–138} However, K metal anodes pose unique challenges due to their larger ionic radius and higher chemical reactivity compared with Li/Na, potentially altering nucleation kinetics and interfacial stability. Future efforts should prioritize these multiscale strategies, explicitly incorporating electrochemical parameters, such as overpotential-dependent nucleation rates and electrolyte concentration effects, to refine K nucleation theory and inform substrate design for uniform deposition.¹³⁹

Filling these knowledge and methodological gaps will be extremely valuable for developing a more predictive and rational approach to stabilize K metal anodes, ultimately accelerating the practical realization of PMBs. In the short term, research should prioritize achieving stable and reversible K plating/stripping through strategic interfacial engineering, substrate design, and electrolyte optimization. Long-term efforts should aim to integrate K metal anodes with high-performance cathodes to enhance cell-level energy density and cycle life. The ultimate objective is to develop full-cell architectures that combine high energy density, extended cycling stability, and scalable manufacturing compatibility, thereby advancing the commercialization of next-generation PMBs for grid-scale energy storage and other demanding applications.

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AUTHOR CONTRIBUTIONS

Conceptualization, Y.H. and Y.X.; formal analysis, Y.H. and P.H.; investigation, Y.H. and P.H.; funding acquisition, Y.X.; supervision, Y.X.; validation, Y.H. and P.H.; visualization, Y.H.; writing – original draft, Y.H.; writing – review & editing, Y.H., P.H., and Y.X.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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