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TOPICAL REVIEW — A 40th Anniversary Celebration: Physics Research and Innovation at Ningbo University

Interstitial electrons in electrides: Multiple electronic regimes and emergent quantum phenomena

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Electrides provide a unique platform for exploring how crystal structure can regulate electronic behavior by controlling the real-space organization of low-energy electrons. Unlike conventional solids, in which electronic states are primarily associated with atomic orbitals and chemical bonds, electrides host interstitial electronic states distributed within crystal cavities, channels, interlayer spaces, or connected void networks. These states establish crystal-structure-defined electronic architectures whose dimensionality, connectivity, filling, and hybridization can be continuously tuned. In this perspective, we view interstitial-electron character as a real-space electronic degree of freedom, describing the structurally encoded organization of low-energy states residing in interstitial regions rather than an independent quantum number. Based on this concept, we classify interstitial electronic states into distinct electronic regimes, including highly itinerant, weakly dispersive or geometry-reconstructed, and strongly hybridized states. These regimes provide diverse platforms for realizing metallic transport, magnetism, ferroic order, superconductivity, topology, unconventional transport, and interfacial electronic-state engineering. We propose a design framework connecting crystal structure, interstitial electronic architecture, electronic regimes, and emergent quantum phenomena, offering a route toward the rational design of quantum materials through real-space electronic architectures.

Keywords: electrides, interstitial electronic states, real-space electronic environments, electronic regimes

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1. Introduction

A central objective in quantum materials research is to identify controllable routes for tailoring electronic states and interactions in order to realize emergent quantum phenomena. Conventional approaches largely achieve this goal through momentum-space engineering, including band-structure design, dimensional reduction, proximity to van Hove singularities (VHSs), and correlation-driven electronic reconstruction.[1,2] While highly successful, these strategies primarily focus on modifying electronic dispersion and band filling. An important complementary question, therefore, arises: can crystal structure regulate electronic behavior by controlling where electrons reside in real space?

Electrides provide a unique platform for exploring this possibility. Unlike conventional solids, in which low-energy electronic states are predominantly associated with atomic orbitals and chemical bonds, electrides host electronic states that extend into the interstitial regions of a crystal lattice, including cavities, channels, and interlayer spaces.[3–5] The resulting interstitial environments vary widely in dimensionality, connectivity, and orbital coupling.[6–8] As a result, electrides provide a fertile platform for exploring a wide range of phenomena, including unconventional transport, topology, magnetism, superconductivity, and ferroic order, in which interstitial electrons may play an important role.[9–12]

Here we use interstitial-electron character as a crystal-structure-defined electronic degree of freedom: a descriptor of how low-energy states are distributed, connected, and hybridized within interstitial regions. Instead of being an independent quantum number, it serves as a complement to orbital, spin, layer, and valley degrees of freedom.

Despite rapid progress in materials discovery, it remains difficult to predict how a given interstitial charge distribution will translate into band structure and collective response. Dimensionality, wavefunction overlap, network geometry, orbital hybridization, and filling act together, allowing interstitial electrons to range from highly itinerant carriers to weakly dispersive or strongly hybridized states. Identifying the structural descriptors that select among these regimes is therefore a central challenge in electride research.

We organize the discussion around real-space electronic-state engineering. As illustrated schematically in Fig. 1, we first discuss how crystal structure creates distinct electronic environments and how these environments influence electronic behavior. We then examine the origin and characterization of interstitial electronic states and discuss how different electronic regimes emerge in electrides. Finally, we highlight

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representative quantum phenomena associated with interstitial electrons and discuss future opportunities for establishing predictive connections between crystal structure, interstitial electronic architecture, and emergent quantum behavior. Viewed from this perspective, electrides provide not only a distinctive materials platform but also a broader framework for understanding how real-space electronic architectures can shape quantum matter.

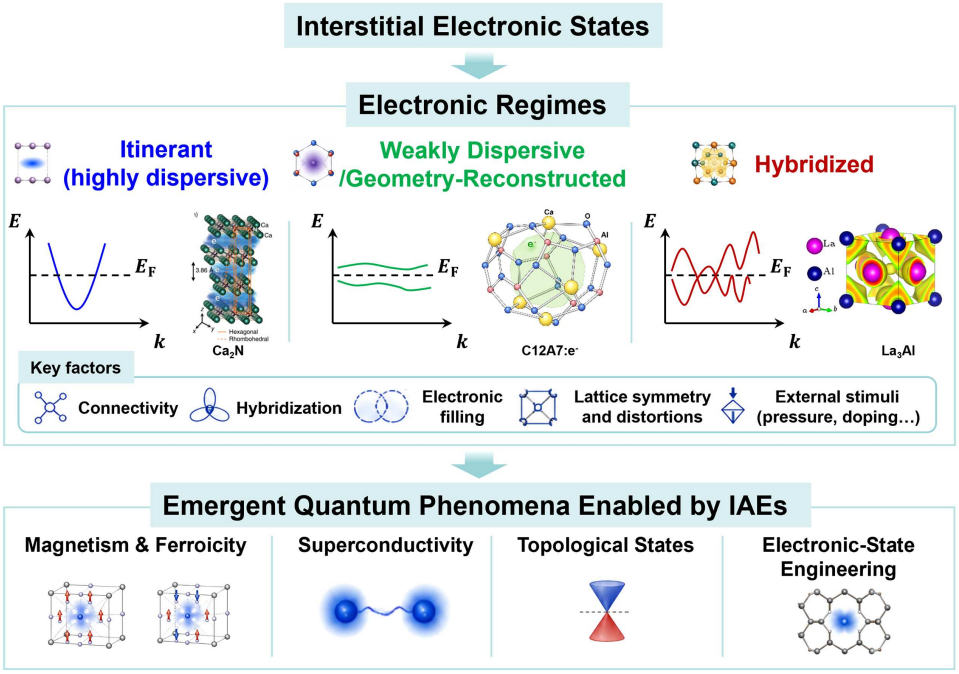

Fig. 1. Conceptual framework of interstitial electronic states as a crystal-structure-defined electronic characteristic. The schematic illustrates the relationship among crystal structure, real-space electronic architectures, electronic regimes, and emergent quantum phenomena, highlighting interstitial electrons as a tunable route for real-space electronic-state engineering.

2. Real-space electronic environments and electronic reconstruction

Electronic behavior in solids is closely linked to how crystal structures organize low-energy electronic states and their interactions. Although electronic properties are commonly described in terms of band structures and Fermi surfaces in momentum space, these quantities originate from the spatial distribution, connectivity, and hybridization of electronic wavefunctions in real space. Crystal structure therefore influences electronic behavior not only by defining atomic arrangements but also by shaping the environments in which electrons reside and propagate. Within a simplified tight-binding picture, the bandwidth can be qualitatively related to the hopping amplitude t and the connectivity of the electronic network z,

$$W \sim zt, \tag{1}$$

where W denotes the bandwidth. Because hopping arises from wavefunction overlap, changes in crystal geometry can modify electronic dispersion through variations in dimensionality, connectivity, and coupling pathways.[13,14] Although this relation captures an important aspect of electronic structure formation, the resulting behavior can also be strongly influenced by factors such as hybridization, electronic filling, and lattice geometry. Understanding electronic behavior, therefore, requires consideration of both momentum-space electronic structure and the underlying real-space organization of electronic states.

From this perspective, a real-space electronic environment encompasses the spatial distribution of electronic states, their connectivity, and their coupling to surrounding orbitals. In conventional materials, low-energy electronic states are primarily described in terms of atomic-centered orbitals and chemical bonds, whereas crystal structures can also create electronically active regions and propagation pathways beyond conventional atomic sites. Such real-space organization determines how neighboring electronic wavefunctions overlap and connect, thereby providing the microscopic basis for variations in hopping, bandwidth, and electronic dispersion. In this sense, crystal structure acts not only as an atomic framework but also as an organizer of electronic architectures in real space.

The influence of such environments can be understood in part through wavefunction overlap and electronic connectivity (Fig. 2(a)). Strong wavefunction overlap and connectivity generally favor broad dispersive bands and itinerant behavior, whereas reduced overlap and connectivity can suppress electronic propagation and narrow the resulting bands. Importantly, real-space electronic environments should be viewed as a framework that constrains, rather than uniquely determines, electronic behavior. Similar structural motifs may sup-

port markedly different electronic properties, while comparable electronic behavior may emerge from distinct real-space environments. As illustrated schematically in Fig. 2(b), variations in electronic connectivity can give rise to markedly different electronic behavior, ranging from highly itinerant states to weakly dispersive electronic structures. In the following sections, we discuss several representative mechanisms through which real-space environments reconstruct electronic states and establish the conceptual foundation for understanding how interstitial electronic architectures emerge in electrides.

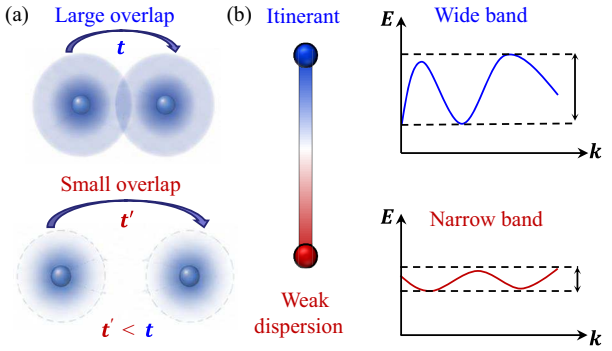

Fig. 2. Real-space electronic connectivity and electronic reconstruction. (a) Schematic illustration of wavefunction overlap between neighboring electronic states, where larger overlap corresponds to stronger hopping amplitude t. (b) Evolution of electronic behavior with changing hopping strength, from itinerant states with broad bandwidths to weakly dispersive states with narrow bandwidths.

2.1. Quantum confinement and dimensional reconstruction

Quantum confinement offers a simple illustration of real-space control over electronic structure. When electrons are confined by external potentials, heterostructures, or layered architectures, their motion becomes quantized along selected spatial directions while remaining itinerant in the unconfined dimensions. Confinement does not necessarily fully localize the electrons; instead, it reduces the available phase space and reshapes the resulting electronic states.

A representative example is provided by quantum wells, where electrons are confined along the out-of-plane direction by potential barriers while remaining mobile within the plane (Fig. 3(a)). Under these conditions, the electronic wavefunction forms standing-wave states along the confined direction, giving rise to discrete subband energies (Fig. 3(b)).[15,16] In the simplest effective-mass approximation, the resulting dispersion can be expressed as

$$E(k) = E_n + \frac{\hbar^2 k_{\parallel}^2}{2m^*}, \tag{2}$$

where E_n denotes the quantized subband energy and $k_{\parallel}$ is the in-plane momentum. The electronic structure therefore becomes highly anisotropic, consisting of quantized out-of-plane states and nearly free-electron-like in-plane dispersion (Fig. 3(c)).[17]

A direct consequence of dimensional reduction is a reconstruction of the density of states (DOS), which evolves from the continuous behavior of three-dimensional (3D) systems to the characteristic step-like profile of a two-dimensional (2D) electron gas (Figs. 3(d)–3(f)).[15] Quantum confinement therefore provides a clear example of how restricting electronic motion along specific directions can generate new electronic structures without necessarily localizing carriers. Although originating from externally imposed potentials rather than intrinsic crystal chemistry, this concept establishes the importance of spatial constraints in determining electronic dimensionality. Related reconstruction mechanisms can also arise intrinsically from lattice geometry and quantum interference, as discussed below.

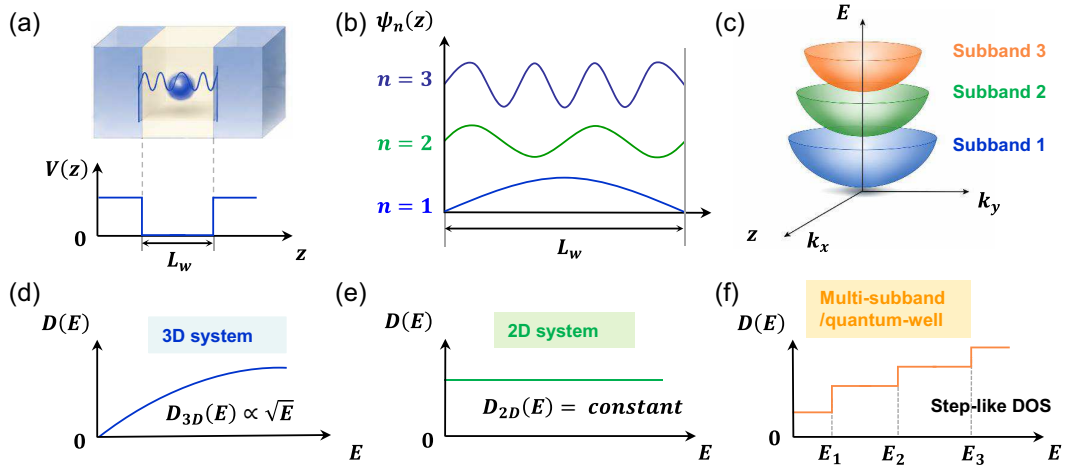

Fig. 3. Quantum confinement and dimensional reconstruction. (a) Electrons confined by an external potential experience restricted motion along one spatial direction. (b) Quantization produces standing-wave states with discrete subband energies. (c) The resulting electronic structure consists of quantized out-of-plane states and nearly free-electron-like in-plane dispersion. (d)–(f) Dimensional reduction modifies the electronic phase space and DOS.

2.2. Geometry-induced electronic reconstruction

Lattice geometry offers a complementary mechanism for reshaping bands in real space. Instead of imposing an external confining potential, geometrically engineered lattices alter connectivity and the available hopping pathways. Representative examples include kagome, Lieb, dice, and decorated lattices (Fig. 4(a)), which host characteristic electronic features such as Dirac dispersions, VHSs, and weakly dispersive flat bands.[18–22] In these systems, the electronic structure emerges directly from lattice geometry rather than external confinement.

The key mechanism is quantum interference among symmetry-related hopping pathways. Within a tight-binding description, the effective propagation amplitude can be viewed as the coherent sum of different hopping processes,

$$t_{\mathrm{eff}} = \sum_n t_n \mathrm{e}^{\mathrm{i}\phi_n}, \tag{3}$$

where t_n and ϕ_n denote the hopping amplitude and accumulated phase along each pathway. Depending on lattice geometry, interference can either enhance propagation or suppress electronic motion along specific directions, producing localized states and weakly dispersive bands.[1]

The kagome lattice provides a prototypical example of geometry-driven electronic reconstruction. Destructive interference around closed hopping loops generates localized plaquette states and nearly dispersionless flat bands, while lattice symmetry can protect Dirac crossings, and the resulting band structure can host van Hove singularities.[20,24–26] The coexistence of dispersive and nearly flat states enhances the DOS and can amplify interaction-driven phenomena. Angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy and spectroscopy (STM/STS) studies of kagome materials such as CoSn and FeSn have experimentally revealed these geometry-induced electronic states (Figs. 4(e) and 4(f)).[20,27–29]

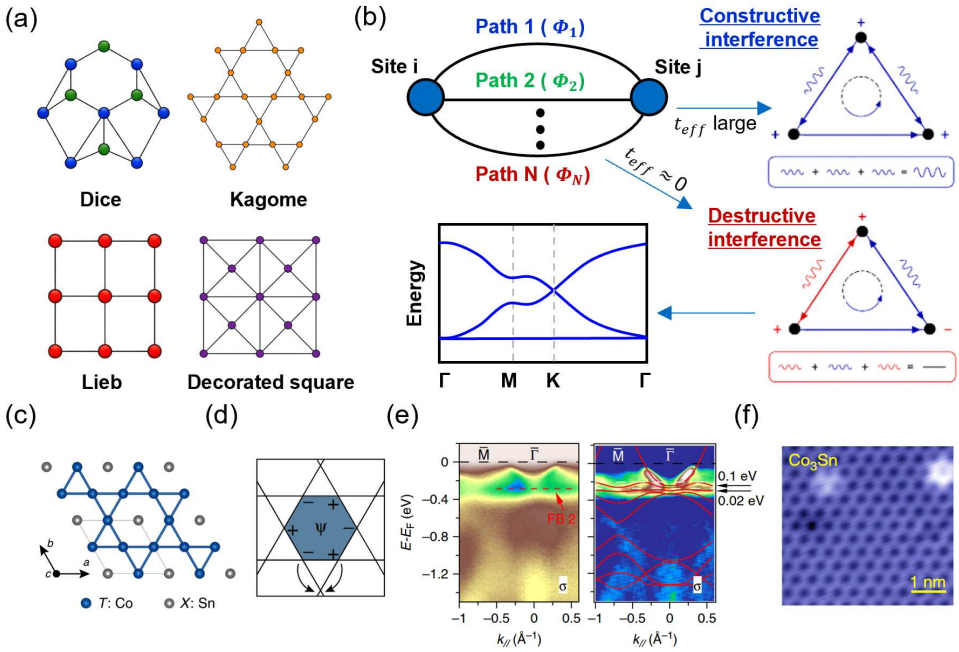

Fig. 4. Geometry-induced electronic reconstruction. (a) Representative lattice geometries, including kagome, Lieb, dice, and decorated lattices. (b) Schematic illustration of quantum interference among multiple hopping pathways. (c), (d) Kagome lattice and the corresponding localized plaquette state.[20] (e) ARPES measurement showing a flat band in CoSn. (f) STM image of a kagome lattice.[29]

Geometrically engineered lattices therefore reconstruct bands through connectivity and interference instead of through dimensional confinement alone. Importantly, lattice geometry constrains, but does not uniquely determine, the resulting electronic structure. This concept is particularly relevant for electrides, where interstitial electrons may themselves organize into geometry-dependent electronic networks.

2.3. Interstitial electronic states in electrides

Among the real-space electronic environments discussed above, electrides represent a distinctive case in which part of the low-energy electronic states reside in the interstitial regions of a crystal lattice. These interstitial states can occupy lattice cavities, channels, interlayer spaces, or interconnected void networks (Fig. 5), instead of remaining centered on atomic orbitals or chemical bonds. Unlike quantum-confined systems and geometrically engineered lattices, where electronic reconstruction originates from external confinement or lattice connectivity, electrides provide an intrinsic realization of real-space electronic-state engineering.

Such states commonly emerge in electron-rich frameworks containing electrostatically favorable interstitial spaces. Depending on the geometry of the surrounding ionic framework, these states may form isolated 0D states, 1D chan-

nels, 2D interlayer electron gases, or fully connected 3D networks.[30,31] These distinct architectures determine the dimensionality, connectivity, and hybridization of the interstitial states and therefore strongly influence their electronic behavior.

Here, the term "electronic degree of freedom" does not imply an independent quantum number analogous to spin or valley. Instead, it refers to a structurally encoded electronic variable associated with the spatial distribution, connectivity, and hybridization of low-energy states in interstitial regions. In contrast to conventional orbital or layer degrees of freedom defined by atomic-centered wavefunctions or crystallographic layers, interstitial-electron character is determined by the location and organization of electronic states within the ionic framework. It should therefore be viewed as complementary to conventional electronic degrees of freedom and can couple with orbital, spin, valley, and topological properties.

The essential feature is that the crystal framework itself defines an electronically active network whose geometry and coupling can be structurally manipulated. Accordingly, changing the size, symmetry, dimensionality, or connectivity of interstitial regions modifies wavefunction overlap, hopping, orbital coupling, and filling. These structural changes can shift the interstitial manifold among itinerant, weakly dispersive, geometry-reconstructed, and strongly hybridized regimes.

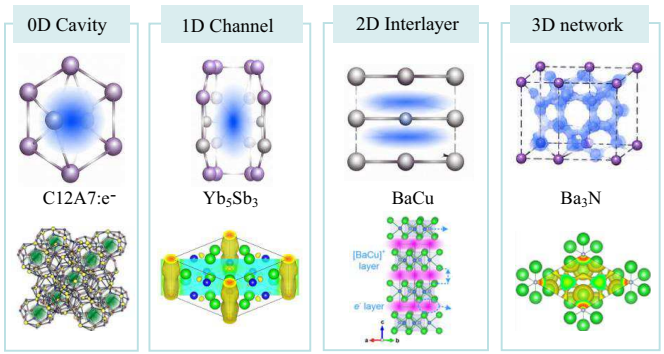

Fig. 5. Dimensional architectures of interstitial electronic states in electrides. Schematic illustrations (top) and representative material realizations (bottom) of (a) 0D cavity-type, (b) 1D channel-type, (c) 2D interlayer-type, and (d) 3D network-type interstitial electronic states.

3. Interstitial electronic states in electrides

3.1. Formation of interstitial electronic states

Interstitial electronic states emerge when crystal structures stabilize low-energy electronic density in regions away from atomic nuclei. In many electrides, electropositive cationic frameworks generate cavities, channels, or interlayer spaces with favorable electrostatic environments, allowing electrons to occupy non-nuclear regions of the lattice.[7,11,32] These interstitial states are therefore not simply excess charge trapped in voids, but electronic states stabilized by the spatial organization of the surrounding ionic framework.

Although the microscopic origins vary among different material families, a common feature is the emergence of low-energy electronic density within crystal interstices. Such states are often described as interstitial anionic electrons (IAEs), emphasizing their electron-rich non-nuclear character.[3,32–34] Their eventual electronic behavior depends on the local geometry, dimensionality, and coupling between interstitial regions and neighboring atomic orbitals.

First-principles calculations and high-throughput searches now find such states across diverse chemistries, structures, and high-pressure phases, indicating that interstitial charge is a broad electronic motif, not a rare exception. Importantly, their formation does not prescribe a specific electronic behavior; instead, it provides the structural basis for multiple electronic regimes.

3.2. Identifying interstitial electronic states

Because interstitial electronic states reside outside conventional atomic orbitals and chemical bonding networks, identifying them requires real-space information in addition to band dispersion. In many materials, dispersive bands near the Fermi level (E_F) may originate from ordinary conduction states, making it difficult to unambiguously establish the presence of interstitial electronic states from electronic dispersion alone. Moreover, because interstitial states can be itinerant, weakly dispersive, or hybridized, no single descriptor is sufficient to fully characterize them. Consequently, the identification of interstitial electronic states typically relies on a combination of complementary real-space and reciprocal-space probes.

Among the available theoretical approaches, the electron localization function (ELF) has become one of the most widely used descriptors for identifying interstitial electronic states.[35,36] ELF characterizes the degree of electron localization in real space and can reveal regions of enhanced localization within lattice cavities, channels, or interlayer regions. It is defined as

$$\mathrm{ELF} = \frac{1}{1+(D/D_\mathrm{h})^2}, \tag{4}$$

where D denotes the Pauli-induced kinetic energy density and D_h is the corresponding quantity for a homogeneous electron gas. The ELF ranges from 0 to 1, with larger values indicating stronger electron localization.[37] In conventional materials, ELF maxima are typically located around atomic nuclei or chemical bonds. In contrast, electrides exhibit pronounced ELF maxima in regions where no atomic nuclei exist, producing non-nuclear maxima (NNMs) that serve as important real-space signatures of interstitial electronic states.[35,38–41]

Beyond confirming their existence, ELF can also provide insight into the dimensionality and connectivity of interstitial

electronic networks. As shown in Fig. 6, high-ELF regions in conventional compounds such as NaCl and MgS are concentrated around atoms and chemical bonds, whereas electrides exhibit distinct interstitial localization.[42] For example, cubic La_3Al displays isolated ELF maxima within empty La_6 octahedral cavities, suggesting spatially localized interstitial electrons, while layered Be_2N exhibits interconnected ELF distributions between neighboring slabs, consistent with a quasi-2D interstitial electron network.[43,44] These examples illustrate how ELF reveals the localization and connectivity of crystal-structure-defined interstitial electronic environments.

To avoid ambiguity arising from a single diagnostic metric, additional theoretical and experimental approaches are often employed. Charge-density analysis, Bader partitioning, and related topological methods can characterize the redistribution of electronic density,[45–47] whereas ARPES and STM/STS provide important reciprocal-space and local probes for assessing the electronic consequences of interstitial states. Low work functions, positron-annihilation measurements, and characteristic transport signatures can further provide indirect evidence for weakly bound interstitial electrons. Used together, these probes provide a more reliable identification than any single metric.

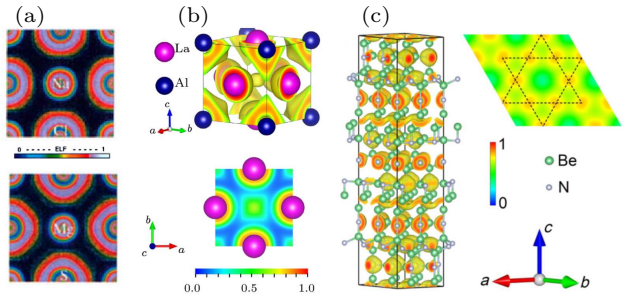

Fig. 6. ELF revealing crystal-structure-defined electronic environments. (a) Conventional ionic compounds NaCl and MgS exhibit electron localization primarily around atomic sites and chemical bonds.[42] (b) In La_3Al, pronounced NNMs appear inside La_6 octahedral cavities, indicating localized interstitial electronic states.[43] (c) In layered Be_2N, interconnected high-ELF regions extend between neighboring slabs, forming a quasi-2D interstitial electron network.[44]

3.3. Electronic regimes of interstitial states

Interstitial electronic states can exhibit markedly different electronic behavior despite sharing a common real-space origin. Depending on connectivity, geometry, hybridization, and filling, these states may form nearly free-electron-like dispersive bands, geometry-reconstructed bands with Dirac or flat-band features, or manifolds strongly mixed with atomic orbitals. Interstitial electrons therefore do not correspond to a single electronic phase, but instead represent a crystal-structure-defined electronic degree of freedom that can manifest across multiple electronic regimes.

3.3.1. Itinerant interstitial states

One important regime occurs when interstitial electrons form spatially extended and electronically connected networks. In this case, the electronic states remain highly itinerant and often exhibit nearly free-electron-like dispersions. Representative examples include layered electrides such as Ca_2N and Y_2C, in which interstitial electrons occupy continuous interlayer regions between positively charged slabs, forming quasi-two-dimensional electron gases.[11,48,49]

Because the interstitial electronic states extend over large spatial regions and retain strong electronic connectivity, the resulting bands remain highly dispersive and cross the E_F. Consequently, these materials exhibit metallic transport, pronounced electronic anisotropy, and relatively low effective masses despite the unconventional real-space location of the electrons. Unlike conventional conduction electrons derived directly from atomic orbitals, these carriers remain spatially separated from atomic nuclei while preserving substantial mobility.

The weakly bound nature of itinerant interstitial electrons underlies several characteristic properties of electrides, including low work functions and efficient charge transfer. In some materials, the coexistence of itinerant interstitial electrons and nontrivial band topology further gives rise to topological electronic states with substantial interstitial character. These examples demonstrate that interstitial states can serve as mobile electronic carriers when the crystal framework provides sufficient connectivity.

3.3.2. Weakly dispersive and geometry-reconstructed states

In contrast to highly itinerant interstitial states, some electrides exhibit reduced interstitial-state connectivity and reconstructed electronic structures. In these systems, the overlap between neighboring interstitial wavefunctions is diminished, leading to suppressed hopping amplitudes and reduced electronic dispersion. As a result, interstitial electrons contribute less directly to metallic transport and may exhibit enhanced correlation effects.

Representative examples include cavity-type electrides such as C12A7:e^-, where interstitial electrons occupy crystallographic voids created by the surrounding ionic framework.[32,50–52] Because neighboring interstitial sites are only weakly connected, the resulting electronic bands are often relatively narrow compared with those found in layered electrides. In such situations, reduced bandwidth enhances the relative importance of electron–electron interactions and can create favorable conditions for correlation-driven phenomena.

Importantly, reduced dispersion does not necessarily imply electronically isolated states. Depending on crystal structure and interstitial-site arrangement, interstitial electrons may

form extended electronic networks with well-defined geometries. In several recently discovered electrides, the interstitial electrons themselves occupy periodic lattice positions and collectively organize into emergent electronic lattices. A representative example is the kagome electride Li_5X (X = Si, Sn), where ELF calculations reveal that interstitial electrons occupy the voids of a lithium framework and form a 2D kagome network (Figs. 7(a) and 7(b)).[53,54] As a consequence, the electronic structure exhibits characteristic kagome features, including Dirac cones, VHSs, and weakly dispersive flat bands (Fig. 7(c)).[55] Similarly, in the layered electride YCl, interstitial electrons form a dice-lattice network (Figs. 7(d) and 7(e)), giving rise to nearly dispersionless bands observed by ARPES (Fig. 7(f)).[21,23,56,57]

These examples illustrate that interstitial electrons are not merely passive charge reservoirs occupying crystallographic voids. Rather, they can themselves constitute emergent electronic lattices whose geometry governs electronic connectivity and quantum interference. In such systems, the resulting electronic structure is determined not only by the degree of dispersion of the interstitial states, but also by the geometry and connectivity of the interstitial-electron network. Consequently, interstitial states can evolve into geometry-reconstructed electronic structures that provide fertile ground for enhanced many-body interactions, unconventional electronic behavior, and emergent ordered states.

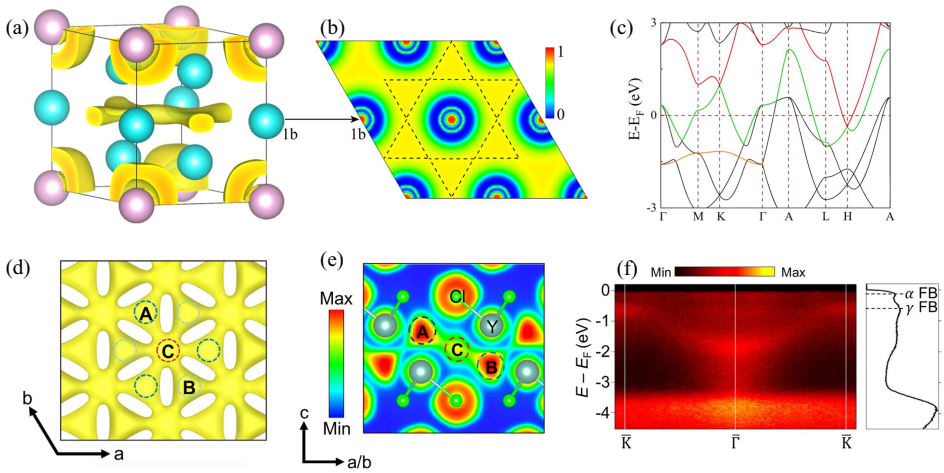

Fig. 7. Real-space organization of interstitial-electron networks and the resulting electronic reconstruction. (a), (b) ELF distributions of Li_5Si showing a kagome-like arrangement of interstitial electronic states. (c) Electronic structure of Li_5Si exhibiting characteristic kagome-derived features.[53] (d), (e) ELF distributions of YCl showing a dice-lattice-like arrangement of interstitial electronic states. (f) ARPES spectrum of YCl revealing weakly dispersive bands near the E_F.[56]

3.3.3. Hybridized interstitial states

A distinct electronic regime emerges when interstitial states strongly hybridize with conventional atomic orbitals. In these systems, the low-energy electronic structure cannot be described solely in terms of isolated interstitial electrons or purely atomic bands, but instead emerges from their mutual coupling. As a result, the electronic behavior is determined not only by the presence of interstitial electrons but also by the strength and character of their hybridization with surrounding electronic states.

A representative example is provided by La_3In. First-principles calculations and ARPES measurements indicate that interstitial electronic states contribute substantially to the low-energy electronic structure while simultaneously hybridizing with La-derived orbitals near the E_F.[58] Consequently, the electronic properties are governed by the coupling between interstitial and atomic degrees of freedom.

Hybridization can significantly modify the dispersion, dimensionality, topology, and interaction strength of interstitial electronic states. In La_3In, interstitial states coexist with nontrivial topological surface states, superconductivity, and anomalous metallic transport behavior.[58–60] The observation of an extended linear temperature dependence of resistivity further suggests unconventional scattering processes within this hybridized electronic environment. Similar behavior may also occur in other electrides where interstitial electrons participate directly in the low-energy electronic manifold and interact strongly with orbital-derived electronic states.[61–63]

These examples illustrate that interstitial electrons should not be regarded as electronically isolated anionic entities. Instead, they can become integral components of complex low-energy electronic structures through hybridization with conventional electronic states. The resulting electronic behavior is therefore governed by the interplay between interstitial-electron character and orbital-derived electronic degrees of freedom.

3.3.4. Structure–electronic regime relationships

The diverse electronic regimes of interstitial states can be understood through a hierarchy of structure-dependent electronic descriptors. Crystal structure defines the real-space architecture of the interstitial regions, including their dimension-

ality, symmetry, geometry, and connectivity. These structural characteristics, in turn, determine the spatial extent and overlap of interstitial wavefunctions, the effective hopping network, the interference between different hopping pathways, the hybridization with atomic-centered states, and the filling of the interstitial electronic manifold. Together, these quantities provide the physical link between crystal structure and the resulting electronic structure.

Dimensionality primarily determines the directions and phase space available for electronic propagation. For example, a two-dimensional interstitial state can exhibit strong in-plane dispersion while remaining weakly dispersive along the out-of-plane direction. The magnitude of dispersion within the allowed directions is instead governed largely by wavefunction overlap and the resulting effective hopping. Strong overlap favors broad dispersive bands, whereas reduced overlap suppresses hopping and promotes weakly dispersive states. Thus, dimensionality and bandwidth are related but distinct aspects of interstitial electronic structure.

The geometry of the electronic network provides an additional route for reconstructing the band structure. Multiple hopping pathways can interfere constructively or destructively, such that electronic networks with comparable connectivity may nevertheless exhibit markedly different dispersions. Geometry-dependent interference can therefore generate characteristic features such as Dirac crossings, van Hove singularities, and flat bands. Hybridization with atomic-centered orbitals provides another important control parameter. Weak hybridization preserves predominantly interstitial character, whereas stronger coupling can transfer orbital character, spin–orbit coupling, exchange interactions, and electron–phonon coupling into the interstitial electronic manifold. Electronic filling further determines which features of the resulting electronic structure are accessed near the Fermi level.

These relationships do not establish a one-to-one correspondence between a structural motif and a particular electronic regime. Extended and strongly connected interstitial networks generally favor itinerant states, whereas reduced overlap and connectivity tend to suppress dispersion. Geometry-dependent interference can reconstruct otherwise dispersive states into Dirac- or flat-band structures, while strong interstitial–orbital hybridization produces mixed electronic states. The resulting behavior also depends on symmetry, spin–orbit coupling, electron–electron and electron–phonon interactions, disorder, and the position of the Fermi level. Interstitial electronic regimes should therefore be viewed as different regions within a multidimensional structure–electronic landscape rather than as strictly separated categories.

This framework also provides a basis for controlling interstitial electronic states. Pressure, strain, chemical substitution, defects, electrostatic doping, and interface construction can modify the geometry and connectivity of interstitial regions, wavefunction overlap, hybridization, or electronic filling, thereby shifting the electronic system between different regimes. Establishing these structure–electronic relationships may therefore enable a transition from the descriptive classification of electrides toward the predictive design and control of their electronic states and emergent quantum phenomena.

4. Emergent quantum phenomena enabled by interstitial electrons

The real-space electronic architectures established by interstitial states provide a new basis for understanding and engineering emergent quantum phenomena. Interstitial electrons can contribute to magnetic ordering, superconductivity, topological electronic structures, and interfacial electronic-state engineering, in addition to serving as charge carriers. The resulting phenomena arise from the interplay between interstitial-state connectivity, hybridization, electronic filling, and coupling to other electronic degrees of freedom. In the following sections, we discuss representative examples illustrating how interstitial electrons support magnetic and ferroic ordering, participate in superconductivity and intertwined quantum states, and enable topological and interfacial electronic-state engineering.

4.1. Magnetism and ferroic order

Magnetism represents one of the most direct manifestations of interaction effects associated with interstitial electronic states. Unlike conventional magnetic materials, where magnetic moments primarily originate from partially filled atomic orbitals, electrides introduce the possibility that interstitial electrons themselves carry spin polarization and participate directly in magnetic ordering. Depending on the degree of itinerancy and confinement, interstitial electrons may support both itinerant and localized magnetic behavior, while recent studies further suggest that they can even serve as carriers of ferroic order.

A representative example of itinerant interstitial-electron magnetism is provided by Y_2C.[64] In this layered electride, positively charged $[Y_2C]^{2+}$ slabs are separated by electron-rich interlayer regions hosting quasi-2D interstitial electrons.[49,65] As shown in Figs. 8(a)–8(d), the interlayer bands exhibit semimetallic overlap near the E_F and undergo spontaneous exchange splitting upon spin polarization, accompanied by a reconstruction of the Fermi surface. The resulting enhancement of the DOS near the E_F drives a Stoner-type magnetic instability and stabilizes an itinerant ferromagnetic state. Importantly, the calculated magnetization density is concentrated predominantly within the interlayer regions

rather than on the Y atoms themselves, as illustrated by the magnetization-density isosurface and cross-sectional maps in Figs. 8(e)–8(g). These results establish interstitial electronic states as an active component of itinerant magnetism, with exchange interactions arising within a spatially extended electronic network beyond localized atomic orbitals.

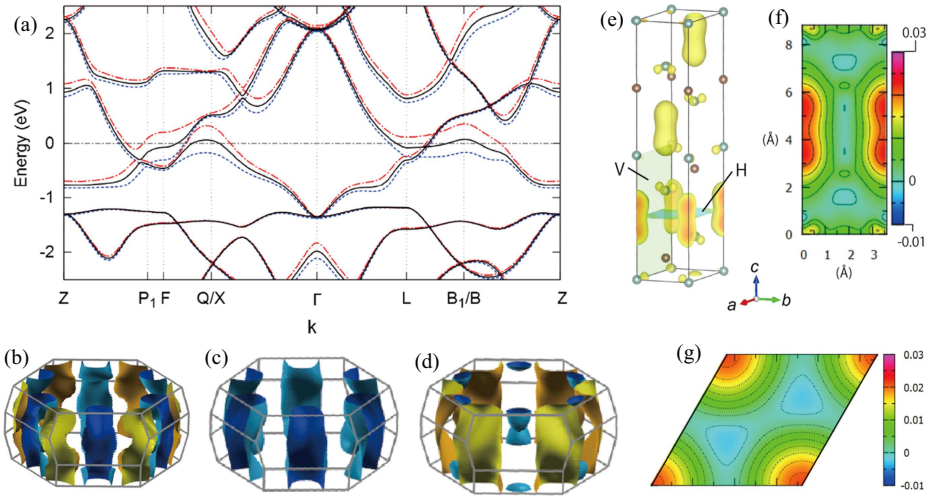

Fig. 8. (a) Spin-nonpolarized and spin-polarized band structures of Y_2C. (b) Fermi surface of the spin-nonpolarized (paramagnetic) state. (c), (d) Minority- and majority-spin Fermi surfaces of the spin-polarized (ferromagnetic) state. (e) Magnetization-density isosurface. (f), (g) Cross-sectional magnetization-density maps.[64]

Stronger confinement can instead favor localized magnetic behavior. Representative examples include $LaBr_2$ and La_2Br_5, where interstitial electrons occupy isolated cavities located at the centers of metal–halogen hexagons.[66] Charge-density and magnetization-density calculations reveal that both electronic localization and magnetic moments are concentrated within these interstitial regions (Figs. 9(a) and 9(b)). Reduced connectivity suppresses electronic hopping and enhances Coulomb interactions, leading to localized magnetic moments and Mott-like insulating behavior. Compared with Y_2C, these systems illustrate how reducing interstitial connectivity can continuously shift the balance from itinerant exchange toward correlation-dominated localized moments.

The role of interstitial electrons extends beyond conventional magnetism. Recent theoretical work on the electride family A_5X_3 (A = Ca, Sr, Ba, Yb; X = As, Sb) suggests that interstitial electronic states can simultaneously support magnetic and ferroic ordering.[45,67,68] As shown in Figs. 9(c) and 9(d), spin density is concentrated almost entirely within interstitial regions, while the atomic framework contributes negligibly to the magnetic moment. The two symmetry-related states AX_+ and AX_- exhibit opposite altermagnetic order and opposite spin-density distributions. Remarkably, switching between these states simultaneously reverses the altermagnetic order parameter and electric polarization (Figs. 9(e) and 9(f)). Because this process occurs through redistribution of interstitial electrons while leaving the atomic framework nearly unchanged, the coupled magnetic and ferroic responses are proposed to arise predominantly from the electronic subsystem itself. These results suggest a fundamentally distinct mechanism of interstitial-electron-driven ferroicity compared with conventional ion-displacement-based ferroic materials.

Taken together, these examples demonstrate that interstitial electrons can support a broad spectrum of ordered states, ranging from itinerant ferromagnetism and localized-moment magnetism to altermagnetism and coupled ferroic orders.

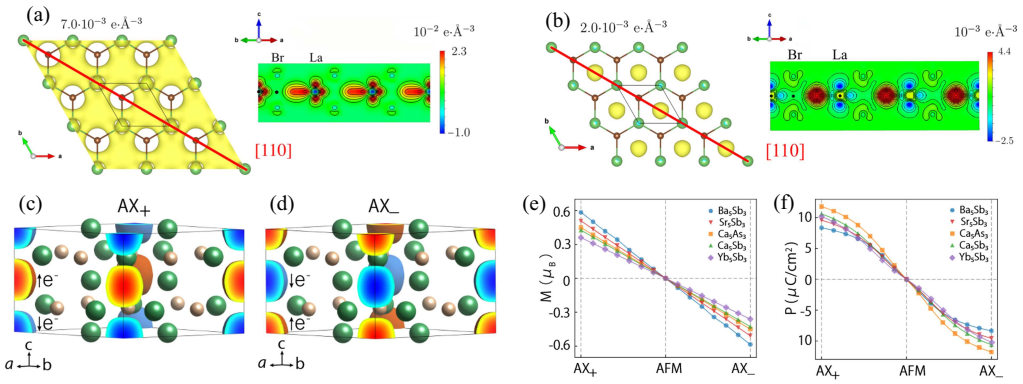

Fig. 9. (a) Charge density corresponding to the band crossing the E_F in $LaBr_2$ and its projection onto the (110) plane. (b) Magnetization density of the ferromagnetic state in $LaBr_2$.[66] (c), (d) Spin-density distributions of Ba_5Sb_3 for the AX_+ and AX_- ground states. (e) Altermagnetic order parameter (M) and (f) electric polarization along the AX_+–AFM–AX_- switching path without spin–orbit coupling (SOC).[67]

4.2. Superconductivity and intertwined quantum states

Superconductivity in electrides does not originate from a single mechanism. Depending on their electronic regime, interstitial states can enhance lattice-mediated pairing, participate directly in the superconducting electronic manifold, or coexist with additional quantum instabilities.

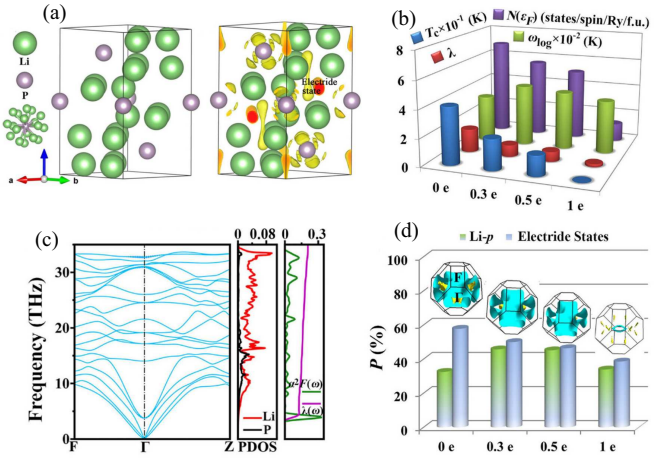

Fig. 10. (a) Crystal structure of R-3m Li_6P at 200 GPa and 3D ELF isosurface. (b) The calculated T_c, λ, ω_{log}, and $N(\varepsilon_F)$ with different hole doping concentrations. (c) Phonon dispersion, projected phonon DOS, $\alpha^2F(\omega)$ and $\lambda(\omega)$. (d) Contribution percentages of electride-states-p and Li-p to $N(\varepsilon_F)$ and the corresponding 3D FS at different doping levels.[69]

High-pressure electrides provide some of the most striking examples. In Li_6P, pressure-induced interstitial electrons form connected dumbbell-like networks (Fig. 10(a)). Hole doping suppresses the hybridized electride-state contribution near E_F, leading to a pronounced decrease in EPC and superconducting transition temperature (T_c) (Fig. 10(b)), together with the disappearance of softened acoustic phonons and an $\sim 87.5\%$ reduction in the EPC constant (Fig. 10(c)). The concomitant reduction of electride-state weight further indicates that interstitial-state-derived electronic states strongly influence the Fermi-surface structure and electron–phonon coupling, thereby affecting superconductivity (Fig. 10(d)).[69]

Another representative high-pressure electride is Li_4Rh. In the $I4/mmm$ phase, interstitial states contribute directly to the low-energy electronic states near E_F and strongly hybridize with Li- and Rh-derived orbitals (Figs. 11(a) and 11(b)). This NNA–atom hybridization is accompanied by strong electron–phonon coupling, as evidenced by the phonon spectrum, the Eliashberg function, and a large EPC constant at 300 GPa (Fig. 11(c)), leading to a predicted T_c of 108.2 K (Fig. 11(d)).[70] These results demonstrate that interstitial electrons participate in the superconducting electronic manifold through their hybridization with atomic states and coupling to lattice vibrations.

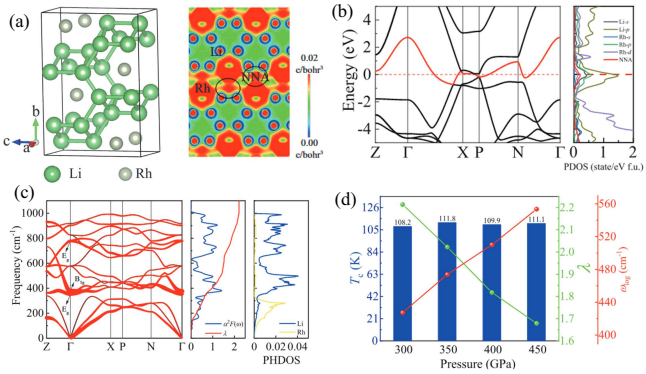

Fig. 11. (a) Crystal structure and partial charge-density distribution near E_F, highlighting the NNAs. (b) Electronic band structure and partial density of states. (c) Phonon dispersion, $\alpha^2F(\omega)$, $\lambda(\omega)$, and phonon DOS at 300 GPa. (d) Pressure dependence of T_c, λ, and ω_{log}.[70]

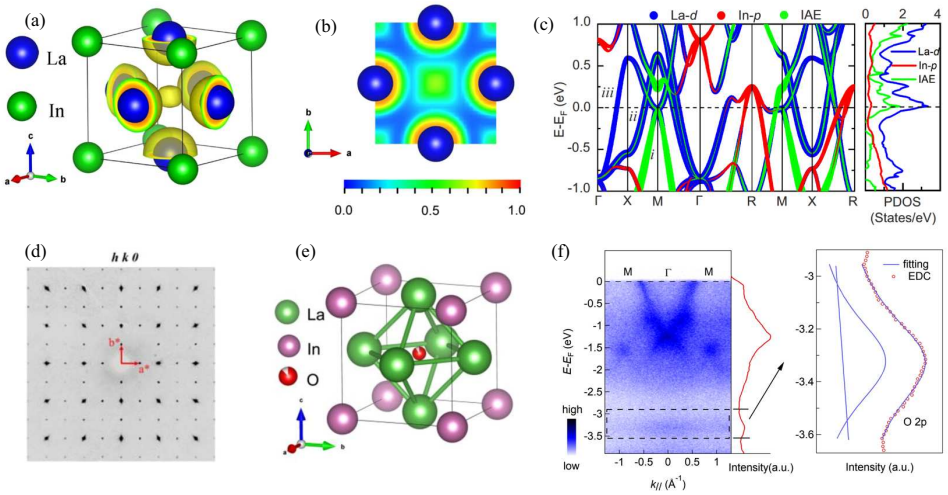

Fig. 12. (a), (b) 3D and 2D ELF distributions of La_3In. (c) Orbital-resolved electronic band structure and partial density of states (PDOS).[58] (d) Reconstructed reciprocal-lattice plane of $La_3InO_{0.9}$. (e) Crystal structure determined from high-resolution XRD. (f) ARPES intensity plot along the Γ–M direction showing O 2p-derived states.[60]

An especially intriguing situation emerges in ambient-pressure superconducting electrides, where superconductivity develops within a strongly hybridized interstitial electronic environment. La_3In provides a representative example. ELF calculations reveal pronounced non-nuclear electron localization within La cages (Figs. 12(a) and 12(b)), while first-

principles calculations and ARPES measurements indicate substantial hybridization between interstitial states and La-derived orbitals near the E_F (Fig. 12(c)). This hybridized electronic environment hosts multiple intertwined quantum phenomena, including superconductivity, a near-E_F VHS, topological Dirac surface states, and strange-metal-like transport behavior. Further evidence for the importance of the interstitial electronic environment is provided by oxygen incorporation studies. Oxygen preferentially occupies interstitial sites associated with interstitial electronic states (Figs. 12(d) and 12(e)), introduces O 2p-derived states (Fig. 12(f)), and strongly suppresses superconductivity, highlighting the sensitivity of the emergent electronic behavior to modifications of the interstitial electronic environment.[60]

Overall, these cases show that interstitial electrons can promote superconductivity through multiple mechanisms and, under suitable conditions, generate complex electronic environments in which superconductivity coexists with topology, VHSs, and unconventional transport behavior.

4.3. Topological states and interfacial electronic-state engineering

Interstitial electronic states can generate diverse nontrivial band structures and, under suitable symmetry and hybridization conditions, support topological electronic states. Depending on the electronic regime involved, topological states may emerge from itinerant interstitial bands, geometry-defined interstitial-electron lattices, or strongly hybridized electronic structures. Representative examples include layered electrides such as Ca_2N and Y_2C, geometry-reconstructed systems such as Li_5Si and YCl, and hybridized electrides exemplified by La_3In. Together, these systems illustrate the wide variety of electronic structures that can arise from interstitial-electron networks.

More importantly, the weakly bound nature of interstitial electrons provides a distinct route for electronic-state engineering. Owing to their low work functions and strong electron-donating capability, layered electrides can serve as intrinsic electron reservoirs that transfer charge efficiently to adjacent materials without introducing chemical disorder.[71] This enables continuous tuning of carrier density and band filling while largely preserving the host crystal structure.

A representative example is the graphene/Ca_2N heterostructure.[72] First-principles calculations reveal efficient transfer of interstitial electrons from Ca_2N to graphene upon interface formation (Figs. 13(a) and 13(b)), producing strong electron doping and a substantial downward shift of the graphene Dirac point (Fig. 13(c)). Importantly, this charge transfer drives the E_F toward a VHS and significantly enhances the DOS. Such behavior illustrates how interstitial electrons can provide a low-disorder route for tuning electronic structure and accessing electronic regimes that are difficult to realize through conventional chemical doping.

More broadly, these examples demonstrate that interstitial electronic states should not be viewed merely as a characteristic feature of a particular materials class. By enabling band-topology design, interfacial charge transfer, and band-filling control, interstitial electronic environments provide a versatile platform for electronic-state engineering and the exploration of emergent quantum matter.

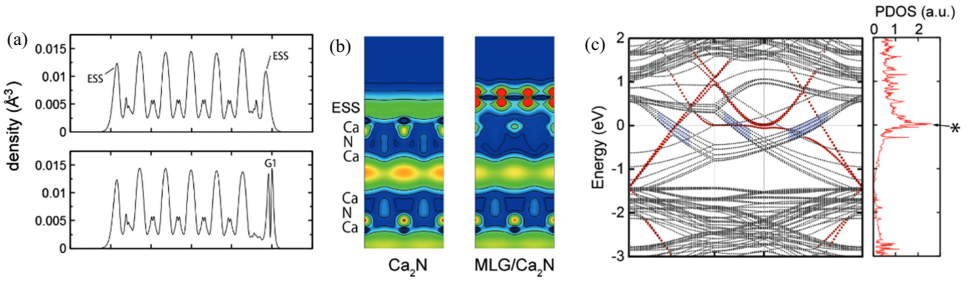

Fig. 13. (a) Partial electron-density distributions of Ca_2N and graphene/Ca_2N heterostructures. (b) Corresponding charge-density contour maps. (c) Calculated band structure and graphene PDOS for the graphene/Ca_2N heterostructure.[72]

5. Challenges and outlook

Despite rapid progress in the discovery and characterization of electrides, a predictive framework linking crystal structures to interstitial electronic behavior remains incomplete. Although numerous materials have been identified to host interstitial electronic states, the criteria determining whether these states evolve into different regimes are still not fully established. Establishing such structure–environment–property relationships represents a central challenge for moving electride research from materials discovery toward rational design.

A second challenge concerns the identification and quantification of the role played by interstitial electronic states. Although tools such as ELF, charge-density analysis, ARPES, and STM/STS provide valuable information, a quantitative understanding of how interstitial states contribute to transport, magnetism, superconductivity, topology, and other collective phenomena remains limited. Future advances will likely require the combination of complementary experimental probes with increasingly accurate theoretical descriptions capable of disentangling the contributions of interstitial and

atomic-centered electronic states. Establishing causal relationships between interstitial electronic states and emergent phenomena, rather than merely identifying their coexistence, will be particularly important for future studies.

Another important direction is the development of reliable strategies for controlling interstitial electronic environments. Pressure, strain, chemical substitution, defect engineering, and heterostructure design have already demonstrated considerable potential for modifying interstitial electronic states and their associated properties. Understanding how these external parameters influence connectivity, hybridization, and electronic filling may provide practical routes for tuning electronic regimes and accessing new quantum phenomena.

Looking forward, electrides may provide a broader framework for understanding how real-space electronic architectures regulate quantum behavior. Establishing general relationships among crystal structure, electronic-state organization, and emergent phenomena may extend these concepts beyond electrides to a wider range of quantum materials.

6. Conclusion

Electrides provide a unique platform in which a portion of the low-energy electronic states resides within the interstitial regions of a crystal lattice. This perspective treats interstitial electrons as a crystal-structure-defined electronic degree of freedom governed by the surrounding real-space electronic environment, beyond their conventional description as unconventional anions or material-specific signatures.

We have discussed how crystal structure can organize interstitial electronic states into different electronic regimes, including highly itinerant states, weakly dispersive or geometry-reconstructed states, and strongly hybridized states. These regimes support a wide range of quantum phenomena, including magnetism, ferroic order, superconductivity, topology, unconventional transport behavior, and interfacial electronic-state engineering. Importantly, these phenomena do not arise from interstitial electrons alone, but from the interplay between interstitial electronic environments, electronic regimes, and many-body interactions.

The key question is therefore not simply whether a compound is an electride, but which interstitial-electron regime it realizes and how that regime can be tuned. Understanding and controlling interstitial electronic environments may therefore provide new opportunities for designing quantum states through real-space electronic architectures.

Acknowledgements

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