Realizing an Electride Lieb Lattice for Emergent Flat-Band Phenomena

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In the pursuit of novel quantum states of matter, condensed matter physicists have long been fascinated by lattice geometries that host flat electronic bands. These bands, characterized by quenched electronic kinetic energy, are a fertile ground for strong electron correlations, leading to a diversity of emergent phenomena, such as unconventional superconductivity, magnetism, and fractional quantum Hall effects.[1] Among these, the Lieb lattice, i.e., a two-dimensional square lattice with a basis of one corner and two edge states, holds a special place with its electronic band structure featuring a massless Dirac cone pierced by a perfectly flat band. However, a significant challenge has persisted for the experimental realization of an intrinsic inorganic Lieb lattice in a real material. Thus far, demonstrations have been largely confined to artificial systems including ultracold atoms in optical lattices,[2] photonic crystals,[3] engineered superlattices on metal surfaces,[4] organic frameworks,[5] and twisted bilayer systems.[6] While these platforms successfully replicate the desired single-particle physics, they often operate at low energy scales or lack the inherent electron–electron interactions necessary to probe the full spectrum of correlated quantum states. The search for a material where the Lieb lattice geometry emerges naturally with its flat band positioned near the Fermi level (E_F) has remained a central goal.

The recent work by Ding *et al.*,[7] published in *Chinese Physics Letters* as an Express Letter, presents a groundbreaking solution to this long-standing problem by introducing the concept of a "Lieb electride". Electrides are a unique class of materials in which electrons are localized in interstitial cavities within the crystal lattice, acting as interstitial quasi-atoms (ISQs) [Fig. 1(a)]. The innovative leap in this study is the proposal that these ISQs, formed by non-bound electrons, can themselves crystallize into a Lieb lattice [Fig. 1(b)]. Using advanced crystal structure prediction MAGUS[8] and first-principles calculations, the authors identify calcium iodide (Ca_2I) as a stable, real-world embodiment of this concept at ambient pressure [Fig. 1(c)]. Crucially, in Ca_2I, the interstitial anionic electrons (IAEs) are not located at the centers of the atomic cages, as in conventional electrides like Ca_2N. Instead, they are pinned at the edges of the squares formed by the calcium atoms. This spatial arrangement directly mimics the "edge site" atoms in the theoretical Lieb lattice model, with the calcium atoms occupying the "corner" sites. This elegant self-assembly of electrons into a desired lattice geometry is a key innovative point that transforms the electride from a mere source of electrons into an active structural component of quantum material itself.

The profound implication of this Lieb lattice formation is the immediate emergence of its characteristic flat bands in the electronic structure of Ca_2I, which generate a pronounced peak in the density of states (DOS) precisely at the Fermi level [Fig. 1(d)]. This direct link between the electride structure and a high, flat DOS at E_F is the catalyst for a remarkable cascade of correlated phenomena. It first triggers a Stoner-type ferromagnetic (FM) instability at ambient pressure, demonstrating that the electride-derived Lieb lattice is a functional system where predicted correlated physics is actively realized.

The true power of this platform is revealed through its tunability under hydrostatic pressure, which drives a sequence of quantum phase transitions. The system evolves from a FM state to a non-magnetic (NM) state at ∼5 GPa, and then to an interlayer antiferromagnetic (AFM) order at ∼17.8 GPa [Fig. 1(e)]. This rich phase diagram underscores a delicate competition between interactions, where increasing pressure enhances Coulomb repulsions and interlayer coupling, ultimately favoring an AFM alignment that allows for greater electron delocalization. Intriguingly, within this high-pressure AFM regime, superconductivity emerges with a calculated T_c of 2.1 K at ∼30 GPa. The study suggests a potential competition between these orders, as the magnetic instability shifts electronic states away from the Fermi level, thereby suppressing the electron–phonon coupling, a hallmark of the complex interplay found in strongly correlated materials.

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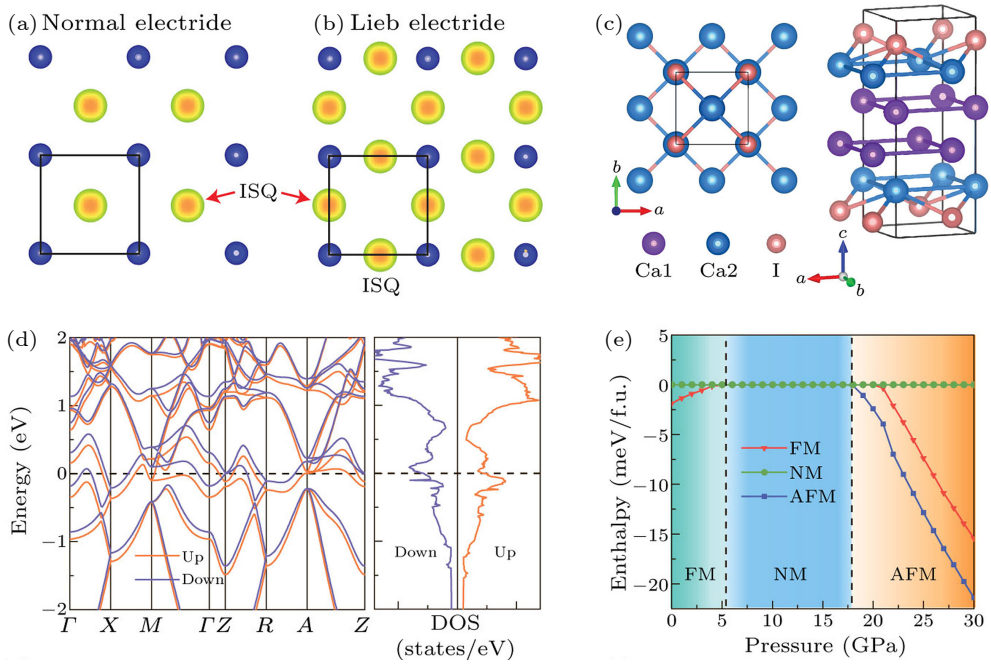

Fig. 1. Lieb electride and emergent flat band phenomena. (a) Normal electride with IAEs at interstitial corners. (b) Lieb electride with IAEs at edge sites. (c) Crystal structure of predicted Ca_2I. (d) Spin-polarized band structure for flat-band induced FM Ca_2I and large DOS at the Fermi level corresponding to the flat band at 0 GPa. (e) Enthalpy difference and phase diagram for NM, FM, and AFM orders. Figures reproduced from Ref. [7], copyright 2025 IOP Publishing.

This work sits at the forefront of several converging trends in condensed matter physics. It aligns with the intense focus on exploring flat-band systems, from twisted graphene layers to kagome metals, for hosting correlation-driven phenomena. The Lieb electride provides a new, intrinsically tunable material class in this landscape. It also significantly expands the scope of electride research. While the recent discovery of a kagome electride in Li_5Si hinted at the potential of ISQs to form exotic lattices,[9] the demonstration of a Lieb electride establishes this as a general and powerful design principle. The "electride design strategy" offers a unique advantage to study flat band-related correlated physics because the lattice sites are themselves composed of electrons, which naturally place the resulting flat bands at the Fermi level, bypassing the common challenge of filling control in atomic lattices.

Looking forward, the implications of this approach are profound. The methodology is not limited to the Lieb lattice; it opens a clear pathway for realizing a whole spectrum of exotic theoretical lattices, such as the checkerboard or pyrochlore, that have remained elusive in solid-state chemistry. The rich phase diagram of Ca_2I under pressure, showcasing a dialogue between magnetism and superconductivity, underscores the potential of these electride systems as highly responsive quantum testbeds. This tunability suggests that future research, leveraging chemical substitution, strain, or electrostatic gating, could precisely manipulate the interplay between these correlated states, potentially stabilizing superconductivity at higher temperatures or unveiling entirely new quantum phases.

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