Beyond Known Archetypes: A Generative AI Framework for Inverse Design of Flat-Band Materials from Geometric Outliers

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Introduction

The quenching of electron kinetic energy in crystal lattices, resulting in flat electronic bands, provides a unique playground for correlated electron physics. When the electronic bandwidth becomes smaller than the Coulomb repulsion, interactions dominate, leading to emergent phases such as unconventional superconductivity, ferromagnetism, and the fractional quantum Hall effect [1, 2, 3, 4, 5]. Historically, the search for these materials has been guided by geometric intuition. We look for specific motifs known to induce destructive interference in the electron wavefunction, such as the corner-sharing triangles of the Kagome lattice, the bipartite structure of the Lieb lattice, or the honeycomb geometry associated with twisted bilayer graphene.

While fruitful, this reliance on known archetypes has created a geometric bottleneck. High-throughput screening efforts often filter databases for these specific sublattices, effectively blinding us to alternative geometries that might support flat bands through different interference mechanisms. The vast space of possible crystal sublattices remains largely unmapped, and we lack a systematic methodology to identify unconventional geometries, which possess the necessary graph theoretical properties for flat bands but do not conform to known crystallographic families. Furthermore, even if a promising abstract graph is identified, the inverse design challenge remains: how to decorate an abstract arrangement of nodes with specific atomic species to realize a stable, synthesizable inorganic crystal.

Here, we present a closed-loop inverse design framework that transcends these well-studied motifs to discover novel flat-band candidates. (i) By stripping known materials down to their fundamental sublattice graphs and training a self-supervised Graph Neural Network (GNN), we construct a latent geometric map that identifies non-canonical topologies, i.e. graphs mathematically distinct from standard families yet physically realizable. (ii) Leveraging the recently developed SCIGEN generative framework [6] to impose structural and chemical constraints on these abstract outliers, we successfully translate unconventional flat-band sublattices into stable inorganic crystals. (iii) We prescreen the generated structures via GNN models depends on stability and flatness, followed by validation through Density Functional Theory (DFT) to discover flat-band materials with out-of-distribution sublattice structures.

Pipeline and main results

We introduce a generative workflow that merges graph representation learning with structural constrained diffusion models. We begin by screening out thousands of flat-band inorganic structures from the Materials Project [7, 8] by the flatness score developed in [9]. The framework is shown in Figure 1. This flatness score is physics-motivated to combine bandwidth and density of states (DOS) signals to give an accurate assessment of band flatness in materials. After the first screening, we extract their constituent sublattices and build tight-binding models to evaluate their potential contribution to destructive interference, similar to [10], and identify the skeletal geometry responsible for destructive interference. These sublattices are fed into a pretrained self-supervised GNN encoder, which learns a continuous latent representation of crystalline topology. By clustering sublattice embeddings and filtering out established crystallographic archetypes, we isolate geometric outliers, which are physically realizable sublattices that reside far from the densely populated latent regions of conventional structures.

Translating these abstract outlier graphs into real materials requires a generative engine capable of handling complex crystallographic constraints. To this end, we leverage the SCIGEN framework [6]. While SCIGEN was originally demonstrated on well-studied geometries, here we utilize its geometric conditioning capabilities to generate chemically plausible crystals around novel outlier sublattices. By denoising the freely variable atoms using the base model while anchoring the constrained skeletons via a predefined trajectory, the diffusion process navigates the conditional chemical space.

We report the discovery of a distinct series of thermodynamically stable inorganic compounds hosting electronic flat bands, derived exclusively from sublattice geometries identified as statistical outliers. We pre-screen generated structures using GNN models for stability and band flatness. Through DFT, we verify that these candidates exhibit dispersionless bands in the vicinity of the Fermi level originating from non-trivial destructive interference pathways absent in standard geometric families. These results demonstrate that the structural phase space supporting flat-band physics is substantially more extensive than the currently cataloged set of crystallographic archetypes.

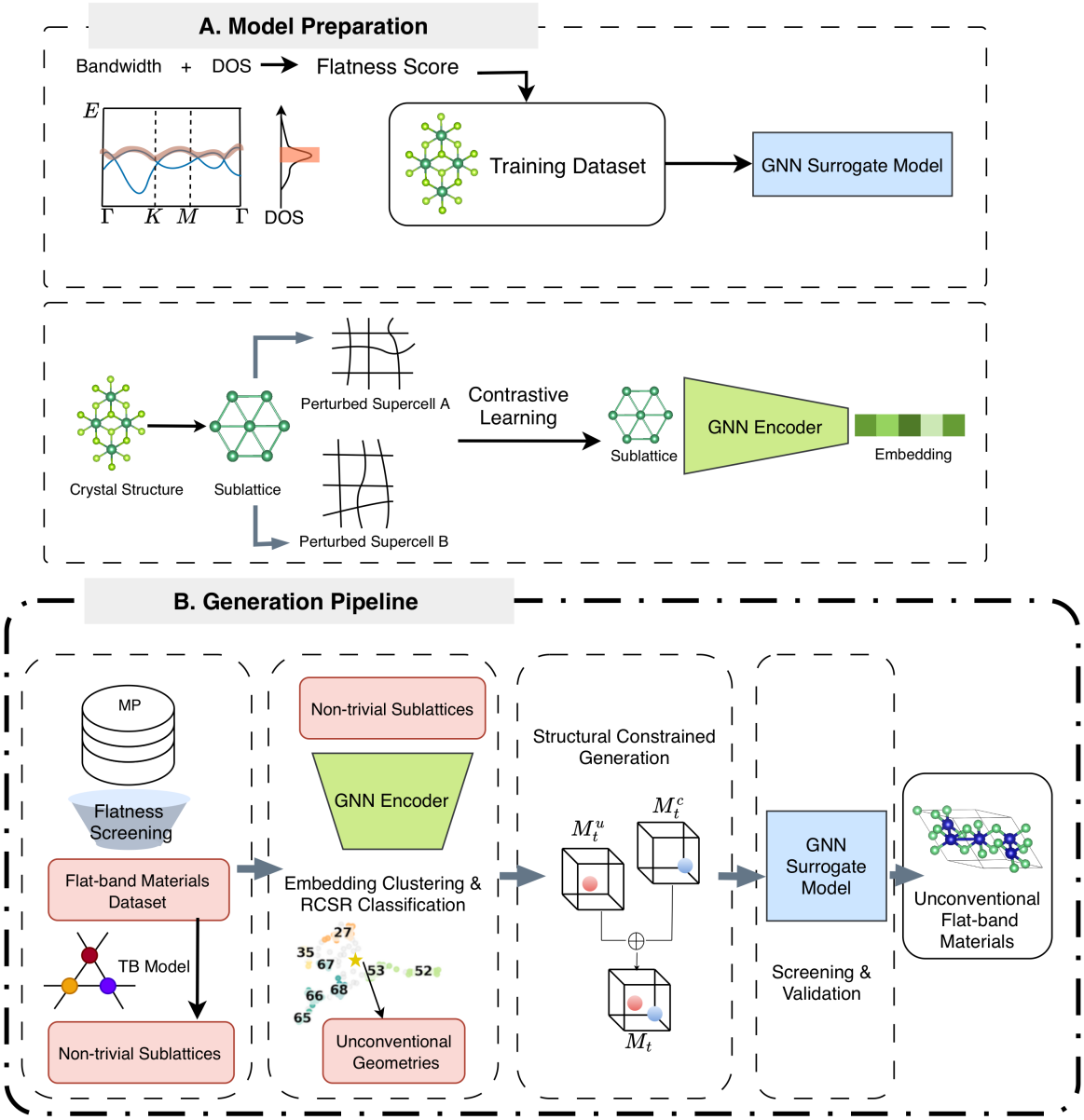

Fig. 1: The framework of generation of unconventional flat-band materials. A. Preparation of GNN models. The training dataset is build by computing flatness score of materials in Materials Project. The GNN encoder used for geometric outlier exploration is prepared through contrastive learning. B. The inverse design pipeline includes four main sections: tight-binding modelling of flat-bands, searching for geometric outliers within embedding space, structural constrained generation and candidate screening and validation.

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