Triviality metric for high-throughput detection of topological flat band materials

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Flat electronic bands form when the kinetic energy of electrons is quenched, making them localised within a region. However, special geometrical features of electronic wavefunctions in certain crystals can create destructive interference that leads to quasi-localised topological flat-band states[1]. The geodesic distance between these quasi-localised flat-band wavefunctions is intrinsically different from the same between trivial and completely localised flat bands[2]. The Fubini-Study metric of wavefunctions, that calculates the geodesic distance, manifests as a complex tensor commonly called the Quantum Geometric Tensor (QGT)[3]. Therefore, calculating the QGT on the wavefunctions can reveal existence of non-trivial delocalised flat bands which can lead to many fascinating many-body quantum phenomena like unconventional superconductivity, ferromagnetism, Wigner crystallisation, etc.

Over the last few years, a large number of attempts were reported towards identifying flat band materials. These studies were mostly inspired by two distinct schools of thought regarding the delocalised flat bands. In the first approach, bipartite, line-graph and split graph lattices are searched in databases [4, 5, 6] since these lattices are known for hosting flat bands with nontrivial topological invariant. The other top-down approach starts the search of both trivial and nontrivial flat band materials from band structures within the computational databases and then attempts to sift the nontrivial flat bands [7, 8, 9]. Although the second approach can potentially identify flat bands which are not included in the list of line-graph and split-graph lattices, there is no straightforward approach to sift the delocalised ones except QGT.

Calculation of QGT on DFT data from databases has a few immediate challenges. QGT is a local metric defined at a k point. Designing a global metric for a lattice based on QGT is a nontrivial task. Secondly, QGT requires calculation of derivatives of wavefunctions on a dense k-grid in the reciprocal cell[10], which is impractical for DFT calculations. To mitigate these issues, we propose a metric defined on the real space to find overlap between real space wavefunction and identify destructive interference as a signature of nontrivial flat bands. It can be calculated in a high-throughput way over a structure graph, yielding a global measure of nontrivial flat bands. The metric is readily usable on spin-polarized and non-spin-polarized DFT calculations and show distinctive characteristics for trivial and nontrivial flat bands.

In this workflow, we first apply an AI-assisted flat band detection algorithm [7] to identify 33000 flat band materials from the Materials Project database. These materials contain both trivial and nontrivial flat bands. The algorithm also identifies the elemental sublattice responsible for the flat band. We then create a structure graph from the supercell of the sublattice structure. Next, we calculate the proposed metric on a discrete grid along the edges of the graph. The connectivity within the supercell helps to calculate nontrivial hopping pathways through flat band states, which can propagate electrons without contributing to kinetic energy. Furthermore, we identify destructive interference as a signature of topological flat bands to confirm the nontrivial nature. Overall, we found only a few thousand nontrivial flat band materials which can contribute to electronic transport from sifting almost 33000 flat band candidates from Materials Project.

Table 1: Snapshot of performance of the triviality metric in identifying delocalized flat bands

Materials Project ID	Formula	Sublattice structure	Density retention score	Destructive interference
mp-20536	CoSn	Co-Kagome	0.28	True
mp-614	NiO2	O	0.0	False
mp-1261	EuZn	Eu-Cubic	0.14	True
mp-1029	BaF2	F	0.01	False

Table 1 and Fig. 1 show snapshot of how the metric scores for typical trivial and nontrivial flat-band materials. For a trivial flat band candidate NiO2, the connectivity among the flat band states makes discontinuous hopping pathways within a unit cell with corresponding 'density retention score' zero. On the contrary, for CoSn, a topological flat-band material, the hopping pathways traverse the unit cell with a 'density retention score' 0.28. We believe that this high-throughput metric can significantly extend the list of interesting flat-band candidates known to us.

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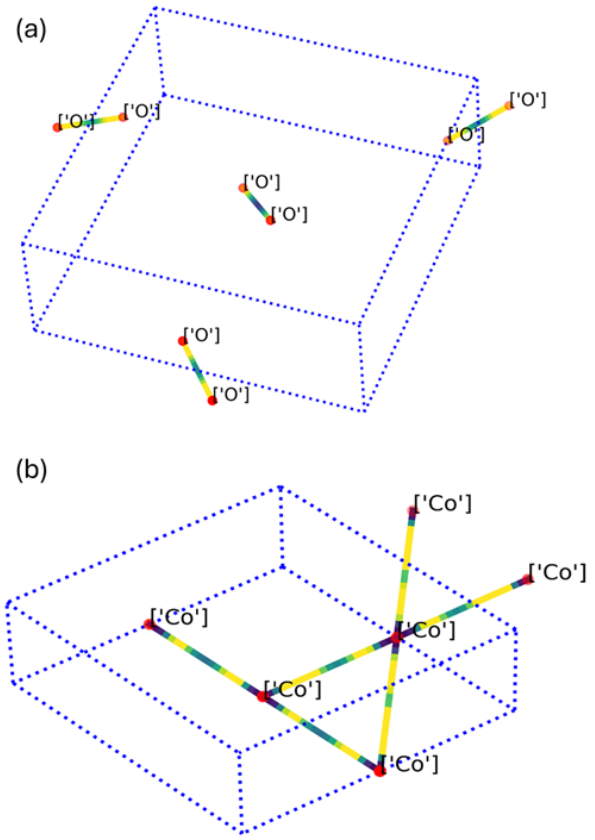

Fig. 1: Graphs of flat band sublattices showing connectivity among atoms in neighboring unit cells: (a) case of oxygen sublattice in a trivial flat band material NiO2 (b) case of Co sublattice in a non trivial flat band material CoSn.

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