Deep Learning Electronic Fingerprints for Mapping Flat-Band Materials in 2D and 3D Databases

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Materials with flat electronic bands often exhibit intriguing properties arising from strong electron-electron interactions. Identifying trends in features of their band structures is crucial for accelerating discovery but is challenging in the vast chemical space of both 2D and 3D materials [1]. We present an unsupervised deep learning framework to efficiently map the electronic properties of flat-band materials in several large computational databases.

Tio this end, a convolutional autoencoder neural network is trained to encode electronic band structures into compact fingerprint vectors. Density-based clustering and visualization techniques then reveal groups of materials sharing similar key features, both structural and electronic.

Applying this approach to 2D flat-band materials uncovers families of compounds with related properties that go beyond known trends [2]. Extending it to the Materials Project database shows the method that robustly captures defining flat-band characteristics in 3D materials as well. The learned fingerprints allow promising unstudied compounds to be readily identified based on their proximity to well-characterized materials in the latent space.

This automated framework provides a powerful, generalizable tool for researchers to rapidly screen computational databases and spotlight compelling 2D and 3D candidates for targeted study. By focusing efforts on the most promising materials, it aims to fast-track the discovery of new flat-band compounds with desirable properties for next-generation quantum and electronic devices.

References

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