Machine learning guided discovery of spin-resolved topological insulators

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Familiar bulk topological invariants of spinful two dimensional insulators, such as the Z2 index or mirror Chern number, indicate the presence of a non-zero (pseudo)spin-resolved Chern number. However, the statement is not biconditional. The spin-Chern number, can survive when these familiar invariants vanish[1]. The identification of solid-state systems hosting a trivial Z2 index and odd spin-Chern number is a pressing issue due to the potential for such compounds to admit band-gaps optimal for use in experiments and quantum devices. Nevertheless, they have proven elusive due to the computational expense associated with their Discovery[2]. This situation motivates the development of new search strategy. Development of a neural network capable of identifying the spin-Chern number is discussed[3]. The resulting neural network is used to guide an ab inito search for colossal band-gap spin-Hall insulators hosting a trivial Z2 index and finite spin-Chern number[4].

References

[1] E. Prodan, Phys. Rev. B, **80,** 125327 (2009)
[2] Tyner et. al, arxiv: 2403.03957 (2024)
[3] Long et. al, npj Comp. Mats. **7** 66 (2021)
[4] Tyner, to appear (2024)

Figures

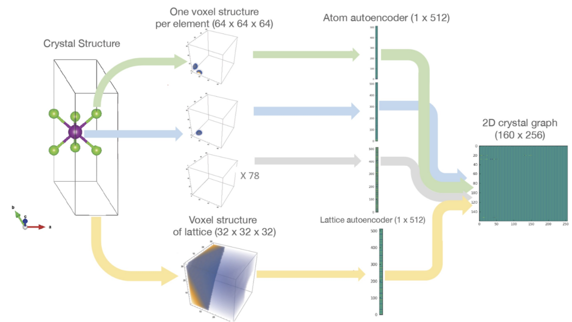

Figure 1. Workflow detailing construction of crystal graphs for continuous representation of lattice to neural network

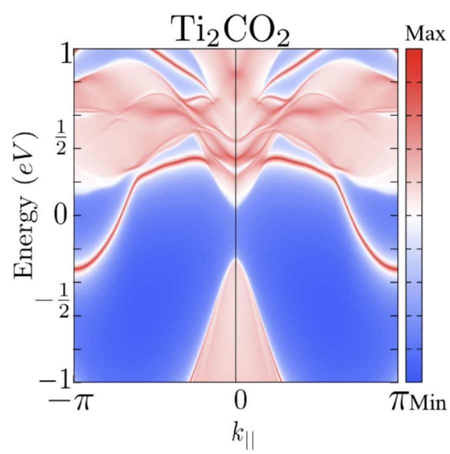

Figure 2. Surface bound modes protected by the non-trivial spin-resolved topology of the bulk as identified by via the trained neural network.