Phase prediction in a honeycomb bilayer structure using ML

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Altermagnets are an emerging class of magnetic materials with promising applications in spintronics [1] and, when combined with superconductors, in topological quantum computing [2]. Altermagnets can exhibit topological Chern insulating phases under certain conditions[3]. Their electronic phases are usually characterised with density functional theory (DFT). DFT is reliable but computationally demanding, which motivates faster approaches to phase classification.

We investigate whether machine learning (ML) can reliably classify phases of an AA-stacked honeycomb bilayer tight-binding model with altermagnetic interactions, as a model-level step towards efficient phase screening.

We compare three types of input. The first is the Hamiltonian parameters. The second is spillage maps, which quantify how spin–orbit coupling changes electronic states across the Brillouin zone [4]. The third is the real-space local density of states (LDOS) at the Fermi level in a ribbon geometry. Samples were labelled by band gap and Chern number. Samples with gaps below $0.1t$ (t: nearest-neighbour hopping) were classified as metallic. An active-learning strategy densely sampled the boundary between topological and trivial insulators. The resulting balanced dataset of about 37,000 samples covers both insulating and metallic phases across several Chern-number sectors.

We benchmarked gradient boosting, fully connected networks, convolutional neural networks, transformers and vision transformers. Our main findings on the test dataset include:

- Topological vs. trivial insulators: gradient boosting on Hamiltonian parameters alone reaches 99.96 % accuracy.
- Single-input transformers (all phases): spillage alone and LDOS alone give 88.5 % and 87.8 %, respectively.
- Combined spillage and LDOS: accuracy rises to 92.8 %, indicating that the two representations are complementary.
- Best multiclass result: 93.4 %, from a feature tokenizer transformer using Hamiltonian parameters.

In the best-performing multiclass models, most errors arise from distinguishing insulators from metals within the same Chern-number group.

These results demonstrate the potential of ML for accurate phase classification in honeycomb bilayer models. Distinguishing insulating from metallic phases remains the main challenge.

References

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