A Symmetry-Aware Multimodal Transformer for Spin Hall Conductivity Prediction

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1. Introduction

Spin Hall materials, which generate spin currents under the excitation of charge currents, play a central role in spintronic devices. Despite their utility, the spin Hall Conductivity (SHC) of commonly used experimental materials remains limited, restricting device performance in critical metrics such as switching speed and energy efficiency. Theoretical studies propose exotic materials with enhanced intrinsic SHC[1], however the systematic discovery of practical candidates faces two fundamental challenges: (1) the lack of a unified physical descriptor linking crystal chemistry to SHC magnitude, and (2) the computational intractability of high-throughput ab initio screening for spin-dependent transport properties.

Recent advances in machine learning have shown promise in spintronics material research, focusing primarily on fundamental properties such as magnetic ground states[2] and thermodynamic stability[3], while the spin-dependent transport properties remain under-explored. Finite studies are limited to specific crystal systems [4], leaving a gap in predictive models for the spin Hall effect (SHE). Momentum-resolved electronic signatures offer critical insights complementary to real-space crystal features [5], yet the integration of reciprocal-space information for spin-dependent property prediction remains largely unexplored, presenting a significant opportunity for further exploration.

Here, we propose a **symmetry-aware multi-modal transformer** architecture to synergistically integrate real-space crystallographic geometry with the reciprocal-space electronic structure descriptors, with crystal symmetry as a prompt. By innovatively incorporating the strength of atomic SOC and valence electron configuration into atomic embeddings and leveraging cross-attention mechanisms, the model achieves effective information fusion between these dual-space representations (Fig.1). The proposed model outperformed the SOTA single-modal GNN model on the unified data set, exhibiting a statistically significant improvement of more than 23%. Extensive validation on independent computational and experimental benchmarks, together with the additional ab initio validation confirmations are performed for additional cross-validation. The proposed approach not only enables SHC prediction but also establishes connections between real-space atomic configurations and momentum-dependent energy dispersion relationship, offering a quantum-aware paradigm for Spin Hall material discovery.

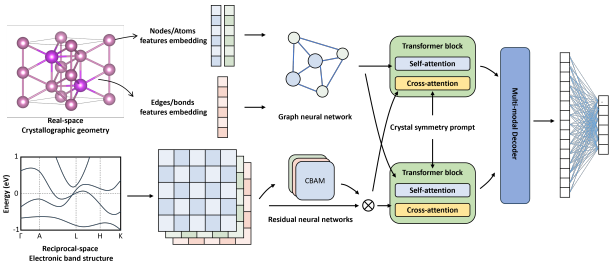

Fig. 1: Overview of the multi-modal Transformer framework for SHC prediction.

2. SHCTransformer

The proposed Physics-guided Multi-modal SHC-Tansformer architecture is composed of three primary components(Fig.1). First, feature extraction modules independently process inputs from the real-space crystal structure (**CS**) and reciprocal-space electronic band structure (**BS**), extracting effective information from the dual-space respectively.

For the **real-space crystal structure**, atomic and bond features are embedded and processed through a graph neural network (GNN) architecture, enabling effective information propagation between nodes (atoms) and edges (bonds). The valence electron configuration and SOC strength information of the composition are creatively integrated into the atomic embedding to supplement the spin-related information of electrons.

For the **reciprocal-space band structure**, feature embedding is achieved using a residual convolutional approach combined with self-attention mechanisms to capture intricate patterns. While acquiring complete band structure information for a material is often challenging, numerous published studies provide accessible band structure images near the Fermi level. These readily available images can

be directly utilized as band structure inputs, significantly simplifying data acquisition and enhancing the accessibility of the model, making it more practical for real-world applications.

These are followed by a transformer-based feature fusion module, which employs cross-attention and self-attention mechanisms to integrate information from both modalities. Specifically, we leverage a standardized representation of the crystal symmetry as a prompt within the cross-attention module. This enables the embedding of symmetry-relevant information during the multimodal fusion process, enhancing the capacity to capture meaningful features.

3. Results and Discussion

The model was trained using approximately 4600 high-throughput computational SHC data from the SHC-DB database[1]. The data is divided into training set, test set and validation set according to the ratio of 8:1:1, and the hyperparameters are fine-tuned on the test set, while the model performance is evaluated using the combination of validation set and test set.

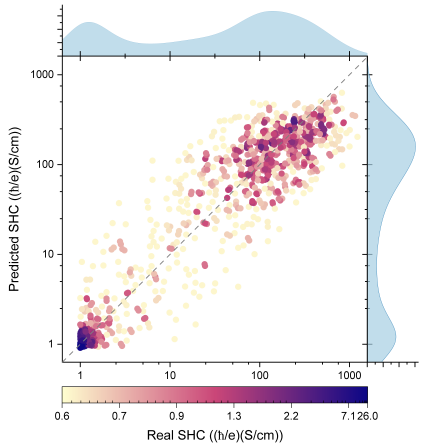

Fig. 2: Overview of the multi-modal Transformer framework for SHC prediction.

First of all, the data of Crystal Structure and Electronic Band Structure modes are used to complete the training respectively, however the performance of the model is not satisfactory. Although single-modality models achieved basic classification between materials with and without finite spin Hall conductivity (SHC), they struggled to predict quantitative SHC values accurately.

The integration of both modalities substantially improved prediction accuracy, achieving a 25% relative enhancement in the coefficient of determination (R^2) compared to best-performing single-modality baselines. As visualized in Fig. 2, the color of each data point indicates the local density of samples in that region. Consistent with the ground truth data distribution, the points are predominantly clustered near zero and around 300 $\hbar/e(S/cm)$, aligning with the two peaks observed in the prediction label distribution shown on the right.

In comparison with state-of-the-art (SOTA) graph neural networks (GNNs)—such as CGCNN, M3GNet, and Gemnet—we observed that models overly focused on pairwise atomic interactions (e.g., bond lengths and angles) underperformed in predicting SHC. This suggests that transport properties such as as SHC may rely more heavily on global symmetry relationships rather than localized atomic environments. A similar conclusion was drawn from traditional machine learning frameworks, such as Matminer combined with Random Forest Regression. Although the predictive performance of ML architecture was limited, the feature importance rankings consistently highlighted crystallographic symmetry-related descriptors as top contributors, further underscoring the critical role of symmetry in SHC prediction.

4. Conclusion and future work

Further efforts will focus on verifying the SHC prediction performance of the model with more theoretical calculation and experimental test data and interpretable analysis. By leveraging dual spatial information—real-space crystal structures and reciprocal-space electronic signatures—the multimodal framework captures a more comprehensive representation of spin transport properties, enhanced by explicit physical symmetry constraints. This approach enables rapid preliminary screening of materials using readily accessible data, prioritizing high-potential candidates for resource-intensive ab initio validation. As a result, the model provides an efficient and scalable pathway to accelerate the discovery of next-generation spintronic materials.

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