УДК 541

PREDICTION OF EXCHANGE BIAS IN MAGNETIC NANOPARTICLES USING MACHINE LEARNING

Капранова К.А. (ИТМО)
Научный руководитель – кандидат химических, Кладько Д.
(ИТМО)

Introduction

The development of advanced magnetic materials is a cornerstone of modern technologies such as spintronics, magnetic storage, and catalysis. A critical aspect of these materials is the exchange bias (EB), a phenomenon resulting from the interaction between ferromagnetic (FM) and antiferromagnetic (AFM) phases in heterostructures. Despite significant research efforts, the design of nanoparticles with optimized EB properties remains computationally expensive and complex. Existing methods, such as density functional theory (DFT) and micromagnetic simulations, offer detailed insights but are limited in scalability and efficiency[1-2]. Recent advancements in machine learning (ML) present a transformative opportunity to overcome these challenges. ML models can integrate experimental data with simulation outputs, enabling faster predictions of EB properties in core-shell nanoparticles. This report highlights the innovative use of ML for predicting EB fields in magnetic heterostructures, focusing on the comparative performance of models like XGBoost and Kolmogorov-Arnold Networks (KAN)[3]. The study also investigates the critical parameters influencing EB behavior, leveraging Shapley additive explanation (SHAP) analysis for interpretability. This work has implications for the rapid discovery of rare-earth-free permanent magnets and other advanced materials.

Main Part

The study's primary objective was to develop and validate an ML framework capable of predicting EB in magnetic nanoparticles. The dataset comprised 980 samples characterized by 37 features, including geometric, magnetic, and crystallographic parameters. The research pipeline began with the collection and processing of data from various experimental studies, emphasizing core-shell structures with FM/AFM interactions[4]. Features such as coercivity, Neél temperature, and magnetic anisotropy were extracted, with missing values addressed using k-nearest neighbor (KNN) imputation methods. This robust preprocessing ensured the quality and reliability of the input data for model training.

Subsequently, several ML models were trained and evaluated, including tree-based ensemble techniques such as XGBoost, random forest, and the Kolmogorov-Arnold Network (KAN). These models were rigorously tested using five-fold cross-validation to ensure their generalizability and robustness. XGBoost emerged as the most accurate model, achieving an R^2 value of 0.75 on the validation dataset, significantly outperforming KAN in general prediction tasks. However, KAN demonstrated exceptional performance in capturing nuanced variations in high EB values, which are critical for specialized applications. This dual approach allowed the study to leverage the strengths of both models, balancing overall accuracy with the ability to detect subtle magnetic behaviors.

The analysis of feature importance, conducted using SHAP, revealed several critical predictors of EB. Coercivity, anisotropy field, and the Neél-to-blocking temperature ratio were identified as the most influential factors. These findings align with established principles in magnetism while also highlighting lesser-known variables, such as Pauling electronegativity, that contribute to EB shifts. The integration of these insights into the ML framework enhances its predictive power and provides valuable guidance for material design. The proposed solution integrates XGBoost and KAN models, creating a scalable alternative to traditional simulations. This approach not only reduces computational costs but also accelerates the discovery of materials with desirable magnetic properties, making it a significant advancement in the field.

The implications of these findings extend beyond the immediate scope of magnetic heterostructures. By elucidating the factors governing EB, this research provides a framework for broader applications in material science, where magnetic properties play a critical role. For instance, understanding the interplay between geometric, magnetic, and crystallographic parameters could inform the development of advanced sensors and energy-efficient magnetic devices. Furthermore, the scalability of the proposed ML models opens pathways for their adaptation to other domains, such as predicting thermal or electrical properties of complex materials, thereby demonstrating the versatility and transformative potential of data-driven approaches in scientific discovery.

Conclusion

This research underscores the transformative potential of ML in the design of advanced magnetic materials. By developing models that streamline the prediction of EB fields, it provides a practical tool for researchers and engineers working on next-generation technologies. The ability to rapidly predict EB properties without relying on computationally intensive simulations accelerates the discovery of rare-earth-free magnets and enhances the precision of spintronic and magnetic storage devices. Furthermore, this study highlights the importance of integrating interpretable ML techniques, such as SHAP analysis, to gain deeper insights into the physicochemical phenomena underlying EB.

Future work should aim to expand the dataset, incorporating a broader range of material compositions and experimental conditions. Exploring advanced deep-learning techniques and hybrid approaches that combine ML with traditional computational methods may further enhance predictive accuracy. Ultimately, this research sets the stage for a new era of data-driven material science, where ML tools play a central role in innovation and discovery.

References

1. Kurichenko, V. L.; Karpenkov, D. Y.; Degtyarenko, A. Y. Experimental and micromagnetic investigation of texture influence on magnetic properties of anisotropic Co/Co3O4 exchange-bias composites. J. Magn. Magn. Mater. 2023, 565 (September 2022), No. 170232. (30)

2. Brown, W. F. Virtues and weaknesses of the domain concept. Rev. Mod. Phys. 1945, 17 (1), 15−19.

3. Wang, R., Yu, H., Zhong, Y., Xiang, H. (2024) Efficient prediction of potential energy surface and physical properties with Kolmogorov-Arnold Networks. *ArXiv Physics*.

4. han, M. H.; Alonso, J.; Khurshid, H.; Lampen-Kelley, P.; Chandra, S.; Stojak Repa, K.; Nemati, Z.; Das, R.; Iglesias, O.; Srikanth, H. Exchange bias effects in iron oxide-based nanoparticle systems. Nanomaterials 2016, 6 (11), 221.