Machine Learning-Assisted Search for Skyrmion-Hosting Heterostructures for Device Applications

S. Grebenchuk [1] **V. Kapitan** [1] **K.S. Novoselov** [1 2] **A. Ustyuzhanin** [1 3]

[1]*Institute for Functional Intelligent Materials, National University of Singapore, 4 Science Drive 2, Singapore 117544, Singapore;* [2]*Department of Materials Science and Engineering, National University of Singapore, Singapore 117575, Singapore* [3]*Constructor University, Campus Ring 1, Bremen, 28759, Germany*. Correspondence to: S. Grebenchuk sergey.gr@nus.edu.sg.

1. Introduction

Magnetic skyrmions are nanoscale, topologically non-trivial spin textures that have attracted intense interest due to their stability, small size, and efficient electrical manipulation. These properties make skyrmions and related topological spin textures promising information carriers for spintronic and unconventional computing architectures. Skyrmions emerge from a delicate balance between competing magnetic interactions, including exchange, magnetic anisotropy, dipolar interactions, and the Dzyaloshinskii–Moriya interaction (DMI). As a result, only a narrow subset of materials and heterostructures can host stable skyrmions, particularly at room temperature and technologically relevant dimensions [1, 2].

In addition to skyrmions being stabilized in certain materials, recent progress has shown that engineered heterostructures, such as metallic multilayers and van der Waals stacks, can also stabilize skyrmionic and other spin textures [3]. However, this flexibility comes at the cost of an enormous design space, where multiple layers, interfaces, and tunable parameters interact nonlinearly.

Machine learning methods offer a powerful route to overcome this bottleneck by guiding simulations toward promising regions of parameter space. Previous studies have demonstrated the possibility of using ML-based classification of magnetic textures or extracting effective Hamiltonian parameters [4], while several works have introduced physics-aware neural networks for micromagnetic simulations as well as neural networks for generative micromagnetic outputs [5, 6]. However, a general and scalable framework capable of handling realistic heterostructures and explicitly targeting skyrmion stability and size is still missing.

In this work, we present a machine-learning-assisted search strategy that tightly integrates micromagnetic simulations with optimization and predictive models. Rather than passively analyzing simulation outputs, the ML models actively goes through the search process, prioritizing configurations that are likely to host stable skyrmions while rejecting undesired magnetic phases. This approach enables systematic discovery of skyrmion-hosting heterostructures across a broad parameter space.

2. Results

The ML-assisted workflow was applied to multilayer heterostructures consisting of two different materials with independently tunable magnetic parameters. Bayesian optimization was used to iteratively propose new simulation points based on previous outcomes, with objective reward functions defined to favor stable skyrmionic states and penalize uniform maze-domain, ferromagnetic, and other phases. Compared to uniform random sampling, the optimizer rapidly converged toward narrow regions of parameter space where skyrmions consistently emerged.

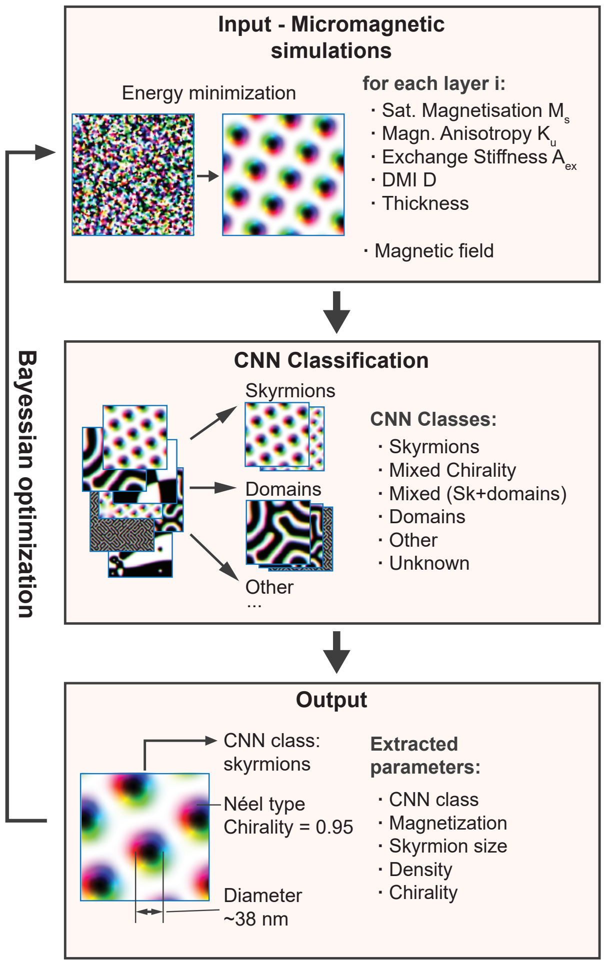

Fig. 1: Bayesian optimization workflow for the search of skyrmion hosting heterostructures based on micromagnetic simulations.

A more detailed workflow is shown in the diagram in Fig. 1, which illustrates the Bayesian optimization procedure for identifying configurations of few-layer heterostructures that favour hosting skyrmions. The optimisation includes multiple steps. First, the micromagnetic simulation with input physical parameters are performed. For each of the layers next parameters are set: saturation magnetization, magnetic anisotropy, exchange stiffness, DMI, and thickness. The magnetic field in the out-of-plane direction is also set. Then, the simulated result is passed through a CNN classification process, in which the class of a spin configuration is determined. So far, several classes were introduced: skyrmions, mixed magnetization and chirality, mixed state of skyrmions and domains, just domains, and others. The CNN was trained on previously simulated data during randomised sweeps, as well as targeted sweeps for a particular class to increase the accuracy of the model. The next step includes additional analysis of the image, which determines characteristics of skyrmions, such as magnetization direction, chirality, skyrmion type (Bloch or Néel), size, density, etc.

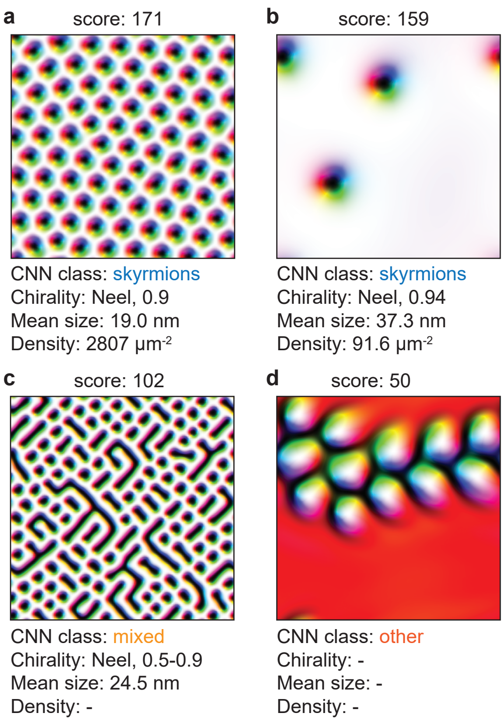

Fig. 2: **Results of Bayesian optimization. a-d** - Examples of Bayesian optimization and final reward scores for different cases of magnetic configurations: skyrmions (a,b), mixed state with both skyrmions and domains (c), and other (d).

Finally, the reward function is calculated, favouring the state with skyrmions, with set preferred sizes, density, and magnetic fields, after which the input parameters for micromagnetic simulations are adjusted, and the process is repeated. The results of the proposed Bayesian optimization are shown in Fig. 2, where examples of two configuration with skyrmions, one for mixed case and one with the class "other", are illustrated.

The next stage involves overlaying the optimized parameter sets onto experimentally accessible materials, identifying candidate compounds with the closest properties to these parameters, and selecting suitable configurations of skyrmion-hosting systems for specific technological applications, such as racetrack memory, artificial synapses, or other spintronic devices. Racetrack memory and related device components can also be further optimized using machine-learning-assisted approaches that systematically refine device geometry and material choice.

3. Conclusion

In summary, this work proposes an ML-assisted algorithm for advanced searching of skyrmionic structures by combining micromagnetic simulations, CNN-based state classification, and Bayesian optimisation. Further correlation of the results with real materials and experimental validation of them can help to advance magnetoelectronic and spintronic technologies that can exploit skyrmions for data processing, transfer, and storage.

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