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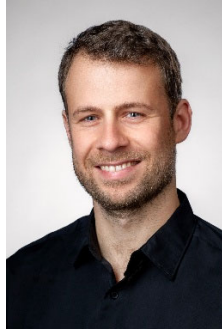


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Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

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Computational magnetic modeling and materials discovery - from DFT to stability properties of skyrmions

Abstract:

The discovery of novel magnetic materials is key to numerous technological advances [1], from energy transition to more capable and energy saving devices for data storage, data processing and quantum computing [2]. The combination of different atomic layers on the nanoscale offers an almost infinite amount of possibilities to fine-tune the magnetic interactions responsible for stability, size and dynamics of magnetic structures, including magnetic skyrmions [3]. While in the past, most breakthroughs were based on experimental trial-and-error discoveries, the community now focuses on better exploration of the material space via computational means [4].

Since magnetism in solid-states is a quantum mechanical effect and the emerging material properties are observed on a larger scale, sophisticated multi-scale approaches consisting of *first-principles* calculations and atomistic simulations are required for accurate predictions. In this talk I am going to present how we achieved this modeling [5, 6], how it compares to experiments [7] and which properties we can extract. Further, the ongoing work of an automated work flow is introduced, utilising this multi-scale approach for high-throughput computations and active learning supported materials discovery.

- [1] B. H. Rimmler *et al.* Nat. Rev. Mat. 10, 109–127 (2025)
- [2] C. Psaroudaki and C. Panagopoulou, Phys. Rev. Lett. 127, 067201 (2021)
- [3] C. Back *et al.*, J. Phys. D: Appl. Phys. 53, 363001 (2020)
- [4] S. Xu *et al.*, npj Comp. Mat. 11, 302 (2025)
- [5] S. von Malottki, Doctoral Thesis, Christian-Albrechts-Universität zu Kiel (2021)
- [6] S. von Malottki *et al.* Phys. Rev. B 99, 060409(R) (2019)
- [7] F. Muckel, S. von Malottki *et al.*, Nat. Phys. 17, 395-402 (2021)