MA 35: PhD Focus Session: Using Artificial Intelligence Tools in Magnetism

Over the last decade, the field of artificial intelligence (AI) has experienced significant growth and progressively offers applications across a wide range of topics, becoming an integral part of our daily lives. Its importance was also underscored by the 2024 Nobel Prize in Physics awarded to John J. Hopfield and Geoffrey E. Hinton 'for foundational discoveries and inventions that enable machine learning with artificial neural networks'. The application of AI methods is also becoming increasingly relevant in research for prediction and data analysis to enhance research, making it faster and more efficient. Typically, these AI tools come from the domain of machine learning, centered on deep learning architectures such as neural networks, convolutional neural networks, and transformer networks. To ensure young researchers, especially in the field of magnetism, can benefit from this progress, we organize the PhD Focus session 'Using Artificial Intelligence Tools in Magnetism'. In this session, experts will demonstrate in highly pedagogical presentations how AI tools can be applied in material science and magnetism. Additionally, there will be a direct, practical introduction to this area of AI tools in magnetism with a hands-on part, where each participant can engage and explore the fascinating world of AI tools for magnetism firsthand using a prepared repository. You can find the repository at https://github.com/kfjml/AI-Magnetism-Session-Regensburg-2025 , please follow the instructions in the Readme, ideally before the session. Alternatively, you can download the repository as a ZIP file, including the instructions in the Readme, from https://download.klaeui-lab.de/AI-Magnetism-Session-Regensburg-2025.

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Time: Thursday 9:30–13:00 Location: H20

Introduction

Invited Talk MA 35.1 Thu 9:35 H20

Artificial Intelligence for Materials Science: Critical Importance of Rare Events, Active Learning, and Uncertainties — •Matthias Scheffler — The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, 14195 Berlin, DE

Materials properties are often governed by an intricate interplay of many processes. As a consequence, the description in terms of meaningful analytical equations is typically inappropriate, and we are promoting the concept of 'materials genes'. These are elemental materials features that 'correlate' with the materials property of interest. Thus, they address the full intricacy and describe (in a statistical sense) the material's property and function.[1]

AI and machine learning (ML) exhibit diminished reliability when entering uncharted data regions. When the training data are representative of the full population (or iid), extrapolation may work. However, for materials this requirement is hardly fulfilled. Still, materials scientists are searching for 'statistically exceptional' situations, and properties are often triggered by 'rare events' that are not or not well covered by the available data, or smoothed out by the ML regularization. This all implies caution when applying ML. In my talk I will explain these issues and routes toward solutions. Key issues are the 'range of applicability' of ML models, the awful overconfidence of prediction uncertainties, and the needs for active learning.

(**) In collab. with Lucas Foppa, Kisung Kang, and Akhil S. Nair.

1) Scheffler M AI guided workflows for screening the materials space. Coshare Science 02, 02 (2024); https://doi.org/10.61109/cs.202403.129

Invited Talk MA 35.2 Thu 10:05 H20

Physics meets data: decoding magnetic inhomogeneities through latent analysis — •Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen

Physicists are trained to simplify complex problems into their fundamental components, often using effective minimal models to describe experimentally observed phenomena. This approach's standard challenges include the difficulty of directly measuring model parameters and the frequent oversimplification or neglect of sample inhomogeneities. As a result, models often fail to make accurate predictions when critical effects are overlooked or inadequately represented. In contrast, data-driven approaches focus on learning directly from the data, ideally without making restrictive assumptions about the data. This talk addresses the problem of hidden features in data and presents computationally efficient, physics-inspired data analysis tools - latent entropy and latent dimension [1,2] - that, for example, allow uncovering magnetic inhomogeneities from video data.

[1] I. Horenko, D. Rodrigues, T. O'Kane, K. Everschor-Sitte, Communications in Applied Mathematics and Computer Science 16, 2 (2021). [2] D. Rodrigues, K. Everschor-Sitte, S. Gerber, I. Horenko, iScience 24, 3 (2021).

Invited Talk MA 35.3 Thu 10:35 H20

AI used for micromagnetic simulations — •Thomas Schrefl[1], Felix Lasthofer[1], Qais Ali[1], Heisam Moustafa[2], Harald Oezelt[2], Alexander Kovacs[2], Masao Yano[3], Noritsugu Sakuma[3], Akihito Kinoshita[3], Tetsuya Shoji[3], and Akira Kato[3] — [1]Christian Doppler Laboratory for magnet design through physics informed machine learning, Wiener Neustadt, Austria — [2]University for Continuing Education Krems, Wiener Neustadt, Austria — [3]Advanced Materials Engineering Division, Toyota Motor Corporation, Susono, Japan

Micromagnetic simulations are an excellent means for prediction of magnetic properties. However, the required computational resources limit the use of micromagnetics for materials design. Machine learning models can serve as surrogate for evaluating target properties during optimization. Artificial intelligence can sort pictures based on content or create new images given keywords. Treating the magnetization distribution as an image, methodologies from image processing can be applied in magnetism. We used this approach to predict the magnetization dynamics of thin film elements. The magnetic states are encoded by a convolutional neural network. For bulk magnets a different approach is required. Their three-dimensional grain structure can be represented by a graph. The regular pixels are replaced by the nodes and edges of a graph. We applied graph neural networks to predict hysteresis properties of permanent magnets. Trained machine learning models can be used for inverse design. Given certain targets, optimized magnets are suggested.

10 min break

Invited Talk MA 35.4 Thu 11:15 H20

Future method for estimating parameters in magnetic films using machine learning — •Kenji Tanabe — Toyota Technological Institute, Nagoya, Japan

Estimating material parameters in fabricated materials is a crucial experiment in the field of materials science. Some parameters are difficult or time-consuming to measure. In spintronics, parameters such as the Dzyaloshinskii-Moriya exchange constant are good examples of this. If these parameters could be easily and quickly estimated, our research field would grow rapidly. Here, we present a new method for estimating parameters in magnetic films from a magnetic domain image using machine learning. A magnetic structure is well-known to be deeply related to magnetic parameters. Although a complicated magnetic structure, which often appears in an as-grown magnetic film, is considered random by human eyes, it is influenced by several magnetic energies. Thus, the characteristics of such parameters are probably hidden in the random magnetic structure. Such a relationship suggests that parameters can be estimated from a magnetic domain image by using pattern recognition. We collected a huge number of datasets of magnetic parameters and magnetic domain images made by micromagnetic simulation and/or taken by magnetic microscopes. The datasets were used as training and test data for the convolution neural network, which is a famous technique in machine learning for pattern recognition. We succeeded in the estimation of the parameters from the magnetic image using machine learning. This result may relieve future researchers from the difficulty of measuring parameters.

MA 35.5 Thu 11:45 H20

Hands-on workshop for using AI in magnetism research — •Kilian Leutner[1], Thomas B. Winkler[2], Jan Maskill[3], Kübra Kalkan[4], and Robin Msiska[4] — [1]Institute of Physics, Johannes Gutenberg-University Mainz — [2]Institute for Molecules and Materials, Radboud University — [3]Department of Physics, University of Kaiserslautern-Landau — [4]Faculty of Physics, University of Duisburg-Essen

In this workshop, participants will receive a practical introduction to applying artificial intelligence (AI) in magnetism research. As a hands-on session, everyone can actively engage. We will demonstrate how to automatically analyze magneto-optical Kerr microscopy images of magnetic skyrmions using AI. The critical and significant step in the analysis involves segmenting the Kerr images using the Skyrmion U-Net, a convolutional neural network [1]. The participants will use their own devices to explore a repository, learning and executing the steps necessary to train and apply a skyrmion U-Net model. The required experimental Kerr data, pre-trained Skyrmion U-Net models, and code are available in a repository at https://github.com/kfjml/AI-Magnetism-Session-Regensburg-2025 or can be downloaded as a ZIP file from: https://download.klaeui-lab.de/AI-Magnetism-Session-Regensburg-2025. Please follow the instructions in the Readme file prior to the session, to make most use of it. This presented approach, is adaptable to other magnetic textures or imaging methods and can also be applied beyond magnetism.

[1] I. Labrie-Boulay et al., Phys. Rev. Applied 21, 014014 (2024)