Modelling and simulation of magnetic materials via AI-driven workflows

Dorye L. Esteras,[*1,2] Jaime Garrido Idea,[2,3] Stephan Roche[1,2,4], Jose Hugo Garcia[1,2]
1 Apeiron Intelligence, UAB Campus, Bellaterra, 08193, Barcelona (Spain)
2 Catalan Institute of Nanoscience and Nanotechnology (ICN2) Campus UAB, Bellaterra, Barcelona 08193, Spain.
3 Universitat Autònoma de Barcelona (UAB), 08193 Barcelona, Spain
4 Institució Catalana de Recerca i Estudis Avançats (ICREA), Spain

* dorye.esteras@icn2.cat, dorye.esteras@apeironai.eu

Computational studies of emergent magnetism have traditionally relied on extensive expert knowledge, manual parameter selection, and case-specific methodological decisions. While individual investigations can achieve remarkable depth, the absence of standardized, reusable, and automated workflows limits reproducibility and renders systematic exploration of complex materials spaces prohibitively costly. As computational materials research increasingly embraces high-throughput screening, data-driven discovery, and closer integration with experiment, the need for structured and automated simulation pipelines has become pressing.

Emergent magnetic phenomena in complex materials continue to drive both fundamental discovery and technological innovation.[1] At the same time, their theoretical description poses significant challenges: magnetic properties are highly sensitive to computational choices and often require consistent coupling between electronic-structure methods and higher-level magnetic models across multiple scales.[2] Over the past decades, advances in simulation techniques have enabled increasingly realistic descriptions, yet their practical application remains labor-intensive and difficult to standardize.

Beyond automation, artificial intelligence (AI) and machine learning are beginning to reshape how simulations of emergent magnetic materials are conducted and interpreted. AI methods can accelerate expensive computational steps, manage methodological complexity, and extract structure from large volumes of simulation data. Surrogate models may replace costly calculations, while data-driven approaches can guide exploration toward physically relevant regions of parameter space. In this context, AI serves as an interface between expert knowledge and large-scale computational infrastructure rather than a substitute for physics-based modeling.

A particularly important role of AI lies in lowering the qualification threshold traditionally required to perform reliable magnetic simulations. By embedding learned patterns and curated best practices within reproducible workflows, machine learning components can support decision-making, detect inconsistencies, and enable adaptive refinement with reduced manual intervention.[3]

In this contribution, I present recent computational studies of magnetic properties in emergent materials using established modeling approaches, emphasizing both scientific results and methodological insights. These case studies motivate a high-throughput effort aimed at constructing a structured database that systematically collects magnetic simulation data together with detailed methodological metadata.

Finally, I discuss the integration of automated workflows into Apeiron, a simulation platform in which AI agents provide an additional layer of execution control and decision support. Artificial intelligence is introduced here as a supporting infrastructure for workflow management and physical modeling.

Overall, this work offers a realistic perspective on the current state of computational research on emergent magnetic materials. It highlights both scientific findings and methodological challenges, and outlines how automation, structured data, and AI-assisted workflows can gradually address long-standing limitations while preserving physical interpretability.

References

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Figures

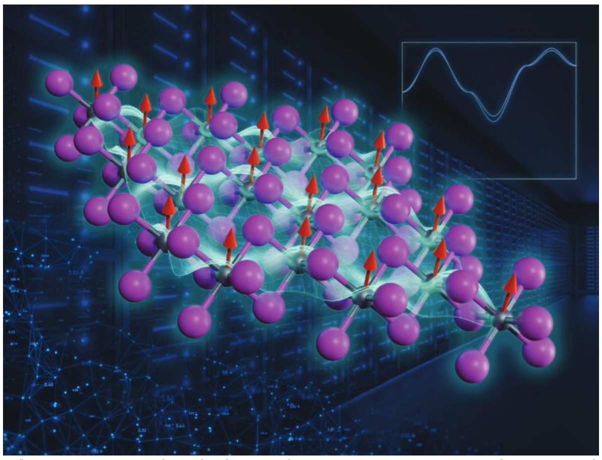

Figure 1. : Simulation of emergent magnetic materials using AI-driven workflows in HPC infrastructures.