Simulation of emergent materials via AI-driven workflows

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Emergent materials have opened new opportunities for fundamental research and technological applications, particularly in the rapidly growing field of two-dimensional (2D) materials.[1] However, the theoretical description, simulation, and optimisation of magnetic properties in these systems remain challenging due to the interplay between reduced dimensionality, strong spin–orbit coupling, exchange interactions, and structural complexity.[2] In this contribution, I will present recent research on 2D magnetic materials, focusing on the key challenges associated with accurately modeling their magnetic behavior across multiple length and energy scales. I will discuss how automated and reproducible computational workflows can significantly accelerate the exploration of emergent materials, enabling systematic studies of stability, magnetic ordering, and transport phenomena. Particular emphasis will be placed on the development of software tools designed to integrate first-principles calculations, atomistic spin models, and data-driven optimisation strategies into unified simulation pipelines. These workflows aim to reduce human intervention, improve scalability, and facilitate the discovery and optimisation of emergent magnetic materials with tailored properties. The presented approach highlights how automation and software development are becoming essential components in modern computational magnetism, bridging the gap between theoretical modelling and materials design for next-generation spintronic applications.

References

1 Gibertini, Magnetic, et al. "Magnetic 2D materials and heterostructures." Nature nanotechnology 14.5 (2019): 408-419.
2 Aldea, J. G., Esteras, D. L.*, Roche, S., & Garcia, J. H. "Challenges and strategies for first-principles simulations of two-dimensional magnetic phenomena." Nanoscale 17.43 (2025): 24955-24989.

Figures

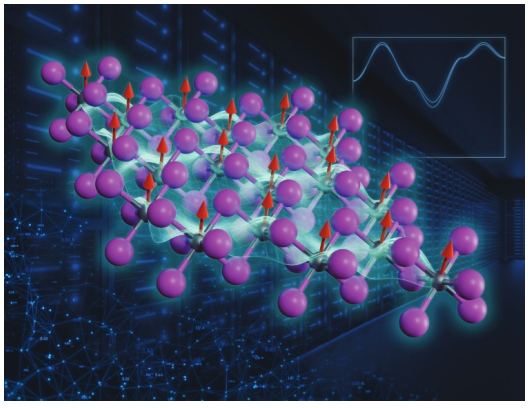

Figure 1: Simulation of emergent magnetic materials in supercomputers