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MSP03: **Interatomic Potentials and Materials Modeling in the Era of Machine Learning**

Organizers: Magali Benoit (CEMES), A. Marco Saitta (LPENS), Nathalie Tarrat (CEMES)
Invited Speakers:

Sponsors: GDR IAMAT

Content:
Over the past decade, machine learning has revolutionized atomistic modeling: interatomic potentials now learn to reproduce *ab initio* energy surfaces with remarkable accuracy while enabling large-scale simulations [1–5]. However, this evolution raises numerous questions. Which physical principles remain essential to embed in these models? How should we balance mathematical structure (equivariance, symmetry, conservation laws) against empirical efficiency? How can we ensure the reliability and transferability of potentials trained on finite datasets? Meanwhile, the emergence of foundation models and large language models (LLMs) for materials, alongside the creation of massive databases, is redefining the roles of knowledge, computation, and interpretation in materials physics. This symposium invites researchers to discuss these open questions, present methodological or conceptual approaches, and explore the intersections of learning, data, and atomistic physics.

Topics Covered:

- Development of machine-learning interatomic potentials (GAP, ACE, NequIP, MACE, Allegro, etc.)
- Equivariant neural architectures and integration of physical symmetries
- Active learning strategies, robustness, and extrapolation
- *Ab initio* databases and FAIR infrastructures for atomistic modeling
- Validation, interpretability, and reproducibility of models
- Foundation models and LLMs applied to chemistry and materials science
- Hybrid approaches combining machine learning and explicit physical laws
- Theoretical, methodological, and epistemological perspectives on data-driven modeling

[1] **Deringer, V. L., Caro, M. A., & Csányi, G.** (2019). *Machine Learning Interatomic Potentials as Emerging Tools for Materials Science*. *Advanced Materials*, 31(16), 1902765.
[2] Unke, O. T. (2021). *Machine Learning Force Fields*. *Chemical Reviews*, 121(16), 10142–10186.

[3] **Ran, N., Yin, L., Qiu, W., & Liu, J.** (2024). *Recent Advances in Machine Learning Interatomic Potentials for Cross-Scale Computational Simulation of Materials*. *Science China Materials*, 67(4), 1082–1100
[4] **Mortazavi, B., Zhuang, X., Rabczuk, T., & Shapeev, A. V.** (2023). *Atomistic Modeling of the Mechanical Properties: The Rise of Machine Learning Interatomic Potentials*. *Materials Horizons*, 10(45), 1956–1968.
[5] **Reinhart, W. F., & Sinnott, S. B.** (2025). *Moving in the Right Direction: Emerging Ideas in Fitting Accurate Potentials*. *MRS Bulletin*, 50(10), 3–9.