Magnetism Meets Machine Learning: Computational Pathways to Novel Materials

Kartsev A. I. [1], * Kushuk L. I. [2]
[1] HSE University, Moscow, Russia
[2] Bauman Moscow State Technical University
Moscow, Russia
*email: akartsev@hse.ru

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This hands-on workshop introduces participants to one of the most dynamic areas in modern physics and materials science: multiscale computational design and analysis of two-dimensional (2D) magnetic materials [1]. The lecture will cover fundamental computational approaches—density functional theory (DFT) [2], Monte Carlo simulations [1], and molecular dynamics (MD)—and demonstrate how recent advances in machine learning (ML) are transforming these methods. Participants will gain an overview of state-of-the-art atomistic simulation tools such as LAMMPS, VASP/Quantum ESPRESSO [3], and Vampire[1], as well as ML-accelerated interatomic potentials (DeepMD, MLIP) that enhance both accuracy and scalability. Core principles of DFT and ML will be discussed in the context of predicting structural, electronic, and magnetic properties of bulk and nanoscale systems, with applications ranging from skyrmion modeling to thin-film growth (CVD/PVD) and thermoelectric phenomena. Designed for a broad audience—including materials scientists, physicists, and engineers—this workshop aims to equip participants with practical insights and computational skills to address contemporary challenges in materials research.

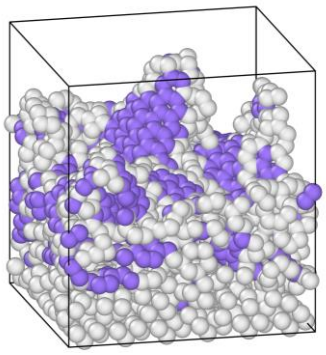

Fig.1 Final atomic configuration obtained using simulated CVD algorithm at 1300 K (grey Si and blue C).

Bibliography

[1] Kartsev, Alexey, et al. "Biquadratic exchange interactions in two-dimensional magnets." npj Computational Materials 6.1 (2020): 150.
[2] Andrade, Xavier, et al. "INQ, a modern GPU-accelerated computational framework for (time-dependent) density functional theory." Journal of Chemical Theory and Computation 17.12 (2021): 7447-7467.
[3] Kartsev, Alexey, Sergey Malkovsky, and Andrey Chibisov. "Analysis of Ionicity-Magnetism Competition in 2D-MX3 Halides towards a Low-Dimensional Materials Study Based on GPU-Enabled Computational Systems." Nanomaterials 11.11 (2021): 2967.