TUT 5: Tutorial: Automated Worksflows (joint session MM/TUT)

Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: H15

Tutorial TUT 5.1 Sun 16:00 H15

Hands-on Tutorial: Automated Workflows and Machine Learning for Materials Science Simulations — •Jörg Neugebauer[1], Tilmann Hickel[2], and Ralf Drautz[3] — [1]MPI für Nachhaltige Materialien, Düsseldorf, Germany — [2]BAM, Berlin, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany

Machine learning techniques in physics and materials science have revolutionized simulations and experimental analysis. Using these techniques to accurately predict, for example, material properties requires the manipulation and use of vast amounts of data. Manual processing and analysis quickly become impractical and error-prone, so the availability of automated workflows is critical to their efficient, reliable, and consistent application.

In this hands-on tutorial, we provide an interactive, practical introduction to workflow management using Pyiron (www.pyiron.org). Pyiron is an integrated materials science development environment based on Python and Jupyter notebooks that can be used for a wide range of simulation tasks, including rapid prototyping, coupling with experiments, and high-performance computing. The tutorial gives a general introduction to the use of Pyiron with a focus on atomistic simulation tasks. As a practical example, all steps of the workflow for the construction of ab initio phase diagrams will be performed interactively by all participants, e.g. the generation of DFT datasets, the training and validation of machine learning potentials as well as the construction of the phase diagram.