MM 1: Hands-on Tutorial: Creating and Running Automated Workflows for Material Science Simulations (joint session MM/TUT)

Time: Sunday 16:00–18:30 Location: H 0104

Tutorial MM 1.1 Sun 16:00 H 0104

Hands-on tutorial: Creating and running automated workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin — [3]ICAMS Ruhr-Universität Bochum, Bochum

Advanced computational simulations in materials science have reached a maturity that allows one to accurately describe and predict materials properties and processes. The underlying simulation tasks often involve several different models and software that require expert knowledge to set up a project and to vary input parameters. The accompanying increasing complexity of simulation protocols means that the workflow along the simulation chain becomes an integral part of research. Effective workflow management therefore is important for efficient research and transparent and reproducible results as also highlighted in the NFDI-MatWerk initiative. In this hands-on tutorial we will provide an interactive hands-on introduction into managing workflows with pyiron (www.pyiron.org). Pyiron is an integrated development environment for materials science built on python and Jupyter notebooks that may be used for a wide variety of simulation tasks, from rapid prototyping to high performance computing. The tutorial will give a general introduction to using pyiron, with a focus on atomistic simulation tasks, followed by the construction of fully ab initio phase diagrams obtained by the training and validation of ACE-machine learning potentials providing a real-life application example.