TUT 3: Hands-on tutorial on workflows for materials science simulation (joint session MM/TUT)

Time: Sunday 16:00–18:00 Location: HSZ 03

Tutorial TUT 3.1 Sun 16:00 HSZ 03

Hands-on tutorial on workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1], and Ralf Drautz[2] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]ICAMS, Ruhr-Universität 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 requires 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.

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 first give a general introduction to using pyiron, with a focus on atomistic simulation tasks. In the second part of the tutorial, the training and validation of ace-machine learning potentials from reference density functional calculations will provide a real-life application example.