TUT 6: Hands on tutorial: Linking large language models with digital workflows for materials science simulations (joint session MM/TUT)

Advanced computational simulations often require chaining several models and software packages together, a process that demands careful workflow management. In this tutorial you can gain hands-on experience with the Python based workflow environment pyiron (www.pyiron.org). 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: TRE/MATH

Tutorial TUT 6.1 Sun 16:00 TRE/MATH

Hands on tutorial: Linking large language models with digital workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]ICAMS, Ruhr Universität Bochum

Advanced computational simulations now reliably predict material properties, but they often require chaining several models and software packages together, a process that demands expert knowledge and careful workflow management. Efficient, reproducible research therefore hinges on automated workflow tools that can handle this complexity. In this tutorial we introduce pyiron (www.pyiron.org), a Python based workflow environment for building and executing fully automated simulation pipelines. We show how complex simulations workflows can be constructed programmatically via Python code as well as via a flow-based graphical user interface. We further introduce how large language models (LLMs) can be embedded to streamline the "human in the loop" tasks. After a brief overview of pyiron's core concepts, we construct workflows for computing ab initio thermodynamic bulk phase diagrams. The necessary steps, such as density functional theory calculations, training ACE-based machine learning potentials, and exploring phase stability using foundational models like GRACE, are all performed within pyiron workflows. Participants will learn how to develop and integrate such workflows into their own materials science simulations, thereby enabling faster, more transparent, and more reproducible research.