Contribution ID: **133** Type: **Poster**

Advancing Digital Transformation in Materials Science: Scientific Workflows within The Platform MaterialDigital

The 'Platform MaterialDigital' (PMD), supported by the German Federal Ministry of Education and Research (BMBF), is spearheading efforts to bundle and coordinate digitalisation within the field of materials science and engineering. Central to its mission are the deployment of decentralised data servers, the adoption of uniform data formats, and the implementation of digital processes through scientific workflows.

As the first funding phase draws to a close, PMD is at a crucial juncture. The groundwork, laid predominantly through academic research, has established a solid foundation. The transition to the second funding phase, now under the leadership of industry-led projects, seeks not only to broaden PMD's impact within the materials science community but also to evaluate the practicality of the developed solutions.

At the heart of PMD's digitalisation strategy are the workflow frameworks pyiron and SimStack, highlighting the platform's commitment to scientific workflows. This presentation will delve into notable advancements within this area, including the integration of semantic data and the semantic characterization of workflows. Furthermore, an overview of the Workflow Store's current status and future trajectory will be provided. This central repository, which offers guidelines for consistent standards in scientific workflows and their components, plays a crucial role in disseminating established workflows and promoting standardization across the community.

Slot length

Primary authors: Dr SCHAARSCHMIDT, Joerg (Karlsruher Institute of Technology); Dr HICKEL, Tilmann (Bundesanstalt für Materialforschung und -prüfung)

Co-authors: Dr STRAUMAL, Alexander (Karlsruher Institute of Technology); BULDIN, Artem (Karlsruher Institute of Technology); Dr REGO, Celso (Karlsruher Institute of Technology); Prof. WENZEL, Wolfgang (Karlsruher Institute of Technology)

Presenter: Dr SCHAARSCHMIDT, Joerg (Karlsruher Institute of Technology)

Session Classification: Poster Session

Track Classification: Research Software: Metadata for Rearch Software