Advancing Digital Workflows in Material Science: Integrating AI into scientific workflows with the MaterialDigital Initiative

Jörg Schaarschmidt [1], Wolfgang Wenzel[1], Jörg Neugebauer [2], Tilmann Hickel [2,3]
[1]Karlsruhe Institute of Technology, Kaiserstr. 12, Karlsruhe, Germany
[2] Max Planck Institute for Sustainable Materials, Max-Planck-Str. 1, Düsseldorf, Germany
[3] Bundesanstalt für Materialforschung- und prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany
Contact@E-mail (Arial 9)

The MaterialDigital initiative is a German funding initiative aimed at driving the digital transformation in material science [1]. Beyond establishing a shared data space and improving semantic data interoperability, an increasing focus lies on the development of interoperable and reusable data-driven workflows. The Platform MaterialDigital (PMD), in collaboration with its funded projects, seeks to standardize scientific data processing through workflows, reinforcing findable, accessible, interoperable, and reusable (FAIR) principles [2].

A central element of this approach is the Workflow Store [3], a repository designed to share, refine, and replicate workflows within the research community. Major challenges within the focus area the integration of experimental workflows, ensuring seamless interaction between computational and laboratory-based data acquisition and processing. Additionally, advancements in Machine Learning (ML) and Artificial Intelligence (AI) play an increasingly crucial role in automating data analysis, optimizing simulations, and enhancing predictive modeling.

We present the latest developments within the Workflow activities of the PMD including the integration of AI-powered methodologies, and the roadmap for overcoming the associated challenges. This contribution highlights the synergy between AI, data-driven workflows, and materials science, paving the way for enhanced reproducibility, collaboration, and innovation in the field.

Figure 1. The Platform MaterialDigital aims at driving digital transformation within material science with the help of funded projects representing various material classes. One focus area is dedicated to developing shared workflow concepts as well as disseminating established workflows via the PMD Workflow Store

References

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