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Advancing Digital Transformation in Material Science: The Role of Workflows within the MaterialDigital Initiative

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The MaterialDigital initiative represents a major driver towards the digitalization of material science. Next to providing a prototypical infrastructure required for building a shared data space and working on semantic interoperability of data, a core focus area of the Platform MaterialDigital (PMD) is the utilisation of workflows to encapsulate data processing and simulation steps in accordance with FAIR principles. In collaboration with the funded projects of the initiative the workflow working group strives to establish shared standards, enhancing the interoperability, and reusability of scientific data processing steps. Central to this effort is the Workflow Store, a pivotal tool for disseminating workflows with the community, facilitating the exchange and replication of scientific methodologies. This paper discusses the inherent challenges of adapting workflow concepts, by providing the perspective on developing and using workflows in the respective domain of the various funded projects. Additionally, it introduces the Workflow Store's role within the initiative and outlines a future roadmap for the PMD workflow group, aiming to further refine and expand the role of scientific workflows as a means to advance digital transformation and foster collaborative research within material science.

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