

Platform MaterialDigital: Enhancing Scientific Collaboration within the MSE Community

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1. Introduction

The 'Platform MaterialDigital' (PMD)[1], supported by the German Federal Ministry of Education and Research (BMBF), focuses on creating a prototypical infrastructure for the digital representation of materials science and engineering. The core of the PMDs approach is enabling digitalization in this field through decentralized data servers, standardized data schemas, and digital workflows. These different aspects are addressed within the platform's focus areas IT architecture, semantic interoperability, and workflows and disseminated via the working group of the focus area community interaction.

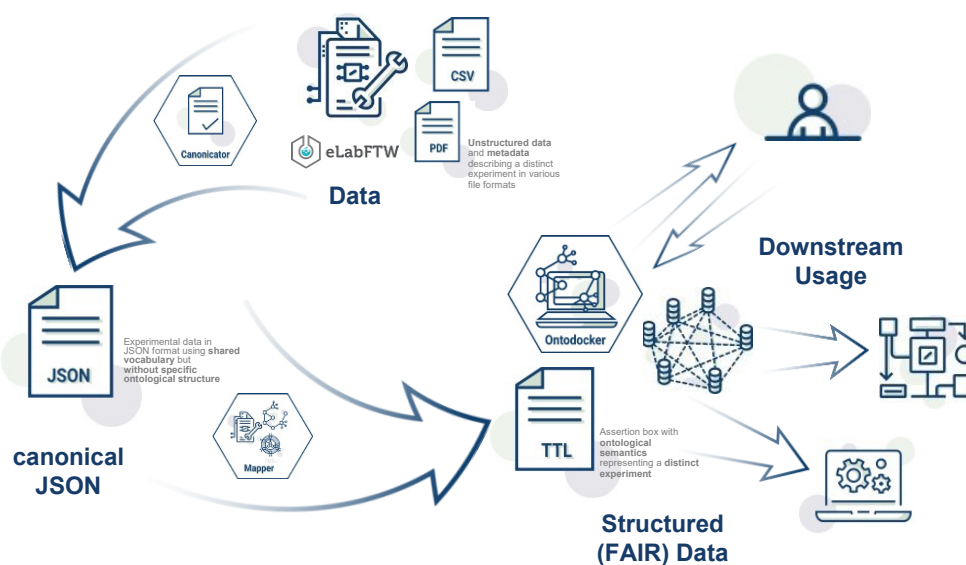


Figure 1: The platform MaterialDigital (PMD) aims to provide prototypical solutions for all processes involved in the digitalization of materials science including acquisition, structuring, storage, and processing of data. The depicted PMD data acquisition pipeline showcases the different concepts involved, including the PMD core ontology [2], in the transformation of raw data to is FAIR-compliant structured data within the context of MaterialDigital.

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2. Scientific Workflows within MaterialDigital

With the first funding phase nearing its end, the PMD is entering a pivotal phase. The initial projects, primarily driven by academic research, have set a robust foundation. The ongoing transition marks the beginning of the second funding phase, now spearheaded by industry-led projects. These new endeavors aim to extend the reach and influence of PMD in the materials science community. At the heart of PMD's strategy to streamline data processing steps and simulation tasks are the workflow frameworks *pyiron* [3] and *SimStack* [4], reflecting the platform's emphasis on scientific workflows. The respective working group focuses on the various challenges involved, including the integration of semantic data and the semantic description of workflows. It Furthermore develops and provides the MaterialDigital Workflow Store [5] as an important tool to spread established workflows and encourage standardization across the community.

3. Conclusions

The Platform MaterialDigital represents a pioneering effort to harness the potential of digitalization in materials science and engineering. By fostering a collaborative ecosystem that bridges academia and industry, the PMD aims to streamline scientific workflows and enhance data interoperability. The transition to industry-led projects signifies a maturation of the PMD's objectives, ensuring that the platform remains at the forefront of innovation and application in MSE. The emphasis on standardized data schemas, decentralized data management, and the integration of semantic workflows underscores the platform's commitment to establishing a comprehensive digital infrastructure. As the PMD moves forward, its continued evolution and the expansion of the MaterialDigital Workflow Store are pivotal in realizing a unified, efficient, and highly collaborative materials science community. By harnessing the collective expertise of the MSE community, the PMD stands not only to enhance scientific collaboration but also to drive forward the development of new materials and technologies. In doing so, it underscores the transformative potential of digitalization in advancing both research and industry.

4. References

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- [4] C. Rego, J. Schaarschmidt, T. Schloeder, M. Penaloza-Amion, S. Bag, T. Neumann, T. Strunk, W. Wenzel; **SimStack: An Intuitive Workflow Framework**. *Frontiers in Materials* 9 (2022) 877597
- [5] <https://workflows.material-digital.de>