Shaping the Future of AI-EnabledDigital Workflows in Material Science

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The MaterialDigital initiative continues to drive the digital transformation of materials science in Germany and Europe by advancing interoperable data spaces, harmonized semantic models, and reusable scientific workflows. Building on earlier developments, current projects contribute application-oriented workflows, metadata patterns, and tooling that increasingly address industrial requirements. Workflows are no longer treated only as technical infrastructure but as enabling technology for producing actionable scientific results, including their use as components within AI-assisted agents and automated analysis pipelines [1,2,3].

Recent developments strengthen Python-based workflow descriptions and portable execution interfaces, supporting consistent integration of laboratory automation, simulation environments, and data services across infrastructures. PMD-X activities complement this by targeting practical interoperability within data-space architectures and by aligning workflow capabilities with emerging European initiatives.

MaterialDigital also contributes nationally and internationally through coordination and standardization activities, including engagement in MADICES and participation in broader community exchanges such as the recent workshops on large language models in materials science. These collaborations strengthen the methodological foundation for AI-supported scientific workflows and promote alignment across community platforms.

This contribution presents current workflow-related activities across the MaterialDigital program, highlights advances in community and industry-oriented projects, and discusses how AI, interoperable workflows, and data-space integration collectively support FAIR scientific practices and accelerate innovation in materials science [1–4]. It furthermore discuses how these concepts will be adressed with the MaterialsCommons4EU project

References

[1] Bayerlein et al., Adv Engin Mat (2024), https://doi.org/10.1002/adem.202401092
[2] Bekemeier et al., Adv Engin Mat, (2025) https://doi.org/10.1002/adem.202402149
[3] https://material-digital.de
[4] https://materialscommons4.eu