MaterialsCommons and FAIR workflows for federated discovery of advanced materials

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Accelerating the discovery, synthesis, and deployment of advanced materials increasingly relies on distributed self-driving laboratories (SDLs) [1] and materials acceleration platforms (MAPs) [2] that tightly integrate simulation, data, and autonomous experimentation. However, the impact of these approaches is presently limited by fragmented infrastructures, heterogeneous data formats, and workflows that are difficult to reuse, compose, or scale across institutions. Here, we present MaterialsCommons, a federated, FAIR-by-design digital infrastructure that addresses these challenges by enabling interoperable, machine-actionable workflows for advanced materials research across Europe [3].

MaterialsCommons provides a multi-node ecosystem with a unified web entry point, comprehensive semantic schemas, and ontology-driven metadata that make materials and process data Findable, Accessible, Interoperable, and Reusable (FAIR) from atomistic simulation to industrial validation. These capabilities are illustrated through federated materials-and-device co-optimization of batteries in FINALES [4], closed-loop, simulation-to-synthesis pipelines such as MODEX and ScatterLab, which autonomously learns synthesis recipes by matching real-time scattering data to simulated patterns [5], and FastCat, an AI-orchestrated MAP that has discovered multi-metal oxygen-evolution catalysts through hundreds of autonomous experiments [6].

Central to MaterialsCommons is the concept of Workflow-of-Workflows (WoW) relying on dynamic workflow managers like PerQueue [7] to call specific computational and experimental nodes in different workflows to create an interoperable network of distributed advanced materials labs [8]. By embedding these capabilities in a governance-backed, sustainably operated infrastructure, MaterialsCommons closes the loop between target structure, autonomous experimentation, and reproducible protocol—while preserving data sovereignty and supporting industrial uptake.

The talk will outline architectural principles, concrete use cases spanning catalysis, batteries, and nanomaterials, and a roadmap toward a pan-European, AI-ready ecosystem for accelerated materials innovation.

References

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Figures

Figure 1. *The MaterialsCommons concept, that will allow materials scientists and engineers to visit a single entry point, and get seamless, secure and interoperable access to data repositories, using a federated infrastructure.*