DARE25-041 - Transforming Research Data into FAIR AI Resources

Abstract

TU Wien produces extensive experimental data across chemistry, physics, and microelectronics, yet much of it remains trapped in proprietary formats and fragmented across local silos, limiting interoperability, reproducibility, and reuse. The dataTUtransform project addresses this critical gap by developing executable, transferable software applications that convert raw laboratory and instrument data into FAIR (Findable, Accessible, Interoperable, Reusable) and AI-ready research resources. The project will focus on representative use cases across key faculties: (1) extraction and structuring of reaction and kinetic data from electronic lab notebooks and measurement instruments in synthetic chemistry; (2) conversion of gas chromatrography-mass spectrometry data from vendor-specific formats into standardized, interoperable resources; (3) export workflows and metadata-rich workflows for microscopy images of surface physics data; and (4) standardized metadata and executable workflows for microelectronic device characterization. All solutions will be developed as open, modular, and reusable code components such as adapters, converters, metadata pipelines and Jupyter notebooks that can be integrated into institutional data environments and extended to other disciplines, thus enhancing data quality, transparency, and reproducibility at TU Wien and beyond.

Scientific disciplines:
General chemistry (25%) | Materials physics (25%) | Data science (50%)

Keywords:
Software interfacesMachine learningFAIR data resources

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Status: Ongoing (01.07.2026 – 30.06.2028)
GrantID: 10.47379/DARE25041

Further links to the persons involved and to the project can be found under
https://www.wwtf.at/funding/programmes/ei/DARE25-041/