

C04: Software Tools for Processing and Contextualizing Materials Characterization Data for FAIR Research Data Management

The quality and quantitative significance of microstructure characterization experiments benefits from a concerted and well-informed usage of different instruments and software tools. Examples include microscopy, spectroscopy, tomography, or mechanical testing of materials.

There is a realized demand and increased interest for storing and processing the metadata and numerical data of such experiments more completely and in better alignment with the aims of FAIR data stewardship principles. While a plethora of data repositories has made tasks like finding and accessing research data easier, tasks like making results more interoperable and reproducible remain a challenge: Different views and expectations about what is considered relevant of an experiment and many different representations provided by software tools need to be more standardized and harmonized to enable true progress.

Therefore, this symposium invites for a cross-community and cross-NFDI-consortia exchange between experimentalists, theoreticians, software developers, and knowledge engineers to exchange about their work within the following topical areas:

- Open software tools and open frameworks which can support experimentalists with data management
- Strategies for including technology partners and scientists to enable a more complete extraction of metadata from commercial software and instruments
- Research and user stories on how to navigate the zoo of file formats and suggestions how to harmonize the pieces of information contained therein.
- Work on electronic lab notebooks and their role in supporting scientists with documenting experiments and adding pieces of information that are not stored in files
- Tools for storing experimental data in repositories and materials science databases
- Application of artificial intelligence in characterization methods
- High-throughput software tools for parameter sensitivity studies that interface with materials databases
- Efficient storage, handling, and management of large-volume/high-dimensional datasets

Symposium Organizer



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