Research Data Management System for CRC/TRR 247

V. Dudarev[1], A. Ludwig[1]

[1]Materials Discovery and Interfaces, Ruhr University Bochum, Bochum, Germany

E-Mail presenting author: alfred.ludwig@ruhr-uni-bochum.de

In the 2nd funding phase of CRC/TRR 247, the INF project develops an extensible, multi-tenant, open-source platform to support research data management in materials science and chemistry. This platform is being created to address multiple requests and related challenges that are being made by various working groups [1]. The platform is based on the native support of chemical entities (chemical systems, compositions) and data objects, and offers users the flexibility to extend and adjust these by a user-defined object type system. The RDMS offers configurable templates for table data and properties for user-defined object types, thereby providing functionality related to efficient storage and flexible search for material science entities. One of the challenges was the recovery of data from the first funding period and their integration into the developed system. This required the extension of the data schema to support the various functional dependencies between the heterogeneous objects found in the original database. We developed a means for edge characterisation, including the links semantics extracted from original data. This was achieved by associating a characterisation object with the oriented edge, which connects two objects in a graph. The improvement enables the modelling and implementation of all types of oriented graphs, which contain objects as vertices and, in turn, could contain a defined properties set or a table data. This provides a solid basis for the modelling of arbitrary materials science domains.

This research was financially supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) Project-ID 388390466-TRR 247 (subproject INF).

[1] V. Dudarev, L. Banko, A. Ludwig, 2024, arXiv:2404.13722. https://doi.org/10.48550/arXiv.2404.13722