The MCL-MAP

A platform for accelerated materials design based on active learning

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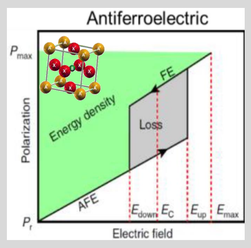
Abstract

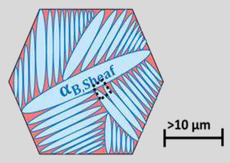
The MCL-MAP is a materials acceleration platform (MAP) based at Materials Center Leoben (MCL), aiming at radically new possibilities for optimizing and discovering high-performance materials. This is achieved by integrating physical modeling and machine learning (ML) in a hybrid modeling approach, where process-structure-property relationships are optimized using an Active Learning Loop (ALL). In more detail, the MCL-MAP includes hard- and software for the platform backbone, a database with FAIR curated data, a framework for running physical modeling and Bayesian optimization algorithms, and a large number of software services for tasks such as interactive analytics, data visualization, data exploration and execution of modeling pipelines. Moreover, it includes a tool for integration of literature that enables search, semi-automated extraction of metadata and digitization of data that are then integrated with the original work. MCL-MAP follows a modular architecture implemented on a container-based infrastructure making it easy to extend and adapt it for future developments. As a proof of concept, the MCL-MAP is currently focusing on two use cases: Bainitic steels with optimized mechanical performance and perovskite-based dielectrics with exceptional energy storage capability. It will be available to cover other materials of interest in the future.

Use cases

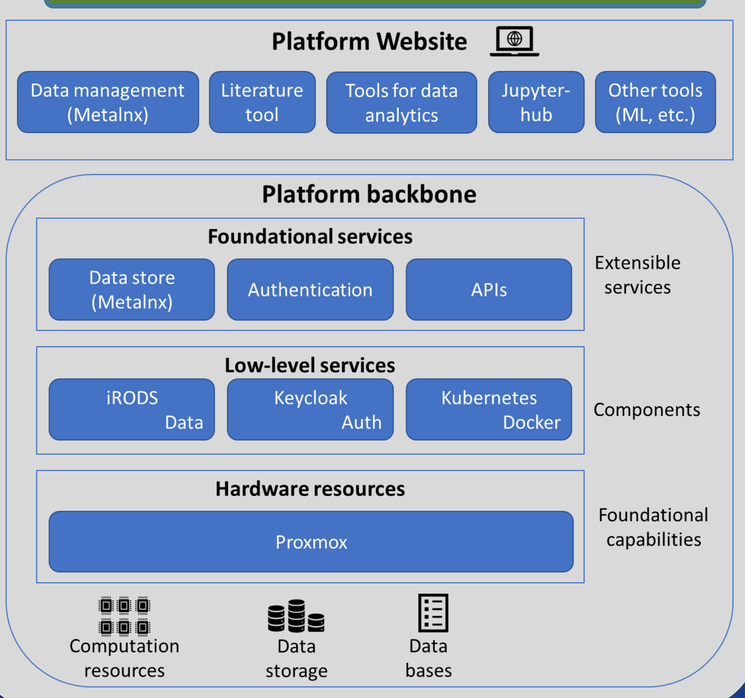
Perovskite (anti-)ferroelectrics: Optimization of energy density of capacitor materials for power electronics (e-mobility, power conversion, etc.)



Bainitic steels: Increase of strength and elongation at fracture (automotive, rails and train wheels, seismic anchors etc.)



Platform Architecture



FAIR database

- iRODS based data storage, ArrangoDB for metadata.
- Unique identifiers for data, use/development of standards for data and metadata.
- Includes data from literature, material production, characterization and simulation.
- Interoperability with other databases and platforms in progress.

The MCL-MAP

Software services
Interactive analytics & visualization
Data exploration; modeling pipelines, Literature tool

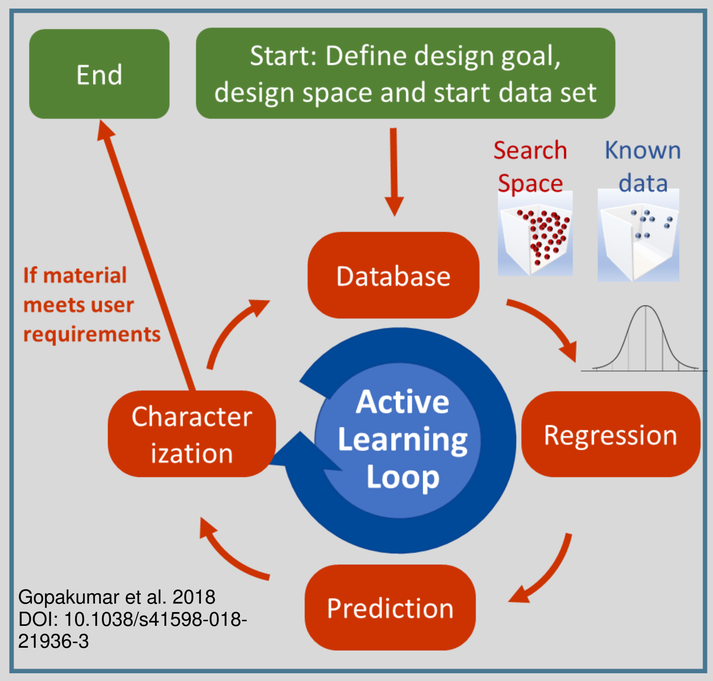
*Framework for **physics based modeling and Bayesian optimization***

FAIR database

Platform backbone

Modular architecture:
Container-based infrastructure → easy to extend and adapt for future developments

Active Learning Loop (ALL)



Software services

Jupyterhub: Script-based analysis, visualization, etc.

Web-based user interfaces for **interactive analytics and visualization** (streamlit).

Modeling and analysis pipelines (Elyra).

Use case specific analysis tools:

- Bainitic steels: Automated detection of Bainite start temperature from dilatometry; austenite fraction from evaluation of XRD peak ratio and dilatation.
- Perovskite dielectrics: Analysis of Raman spectra (combing exp + DFT)

Literature tool

- Automated keyword search/crawler.
- Semi-automated digitation of figures.
- Digitized data and metadata (chemistry, processing) stored together with original papers.
- Search for data and metadata on same footing as for bibliographic data.

*Framework for **physics based modeling and Bayesian optimization***

- The MCL-MAP integrates physics based models, materials data and tools for Bayesian optimization
  → ecosystem for the ALL

Bainitic steels:

- Multi-dimensional parameter space including composition and heat treatment
- Hybrid model combining physics-based and ML approaches (e.g. Gaussian Process Regression).
- Bayesian inference for choosing best parameters for modeling the bainite start temperature.
- Optimization of Pareto front of yield strength and uniform elongation.

Perovskite (anti-)ferroelectrics:

- Probabilistic hybrid models under development.

Summary

- MCL-MAP enables active-learning based materials optimization.
- Integration of platform backbone and web services, FAIR data, physics-based , ML models.
- It is being developed by MCL, Know Center Graz and Montanuniversität Leoben together with use case specific partners.

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