The MCL-MAP

A platform for accelerated materials design based on active learning

Jürgen Spitaler[1], Daniel Scheiber[1], Natalia Bedoya[1], Han Tran[2], Heimo Gursch[2] and Lorenz Romaner[3]

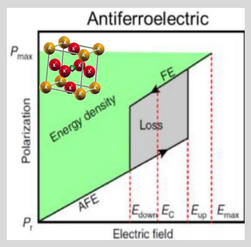
(1) Materials Center Leoben Forschung GmbH, Leoben, Austria (2) Know Center, Graz, Austria (3) Montanuniversität Leoben, Leoben, Austria

Abstract

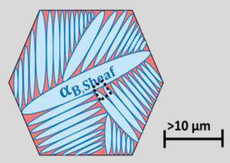
The MCL-MAP is a materials acceleration platform (MAP) based at Materials Center Leoben (MCL), aiming at radically new possibilities for optimizing and discovering high-performance materials. This is achieved by integrating physical modeling and machine learning (ML) in a hybrid modeling approach, where 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

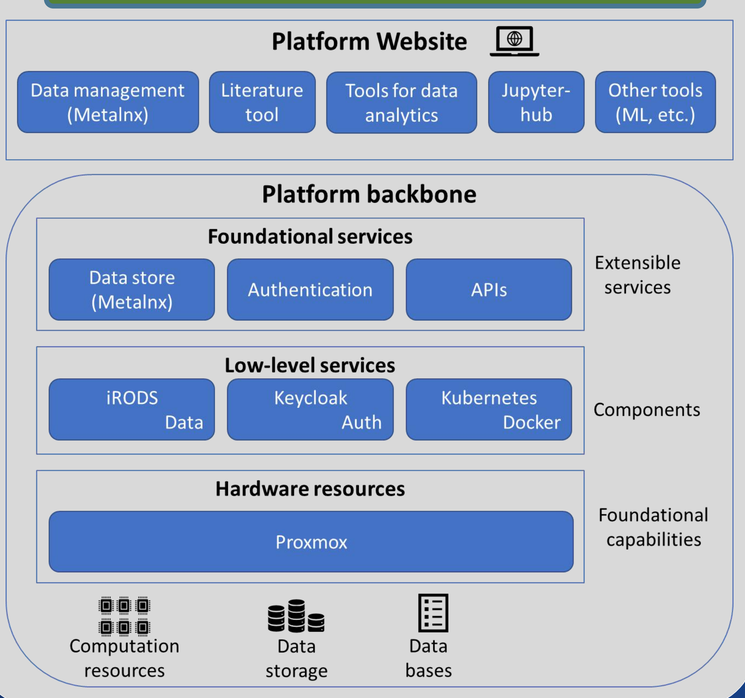
Perovskite (anti-)ferroelectrics: Optimization of energy density of capacitor materials for power electronics (e-mobility, power conversion, etc.)



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

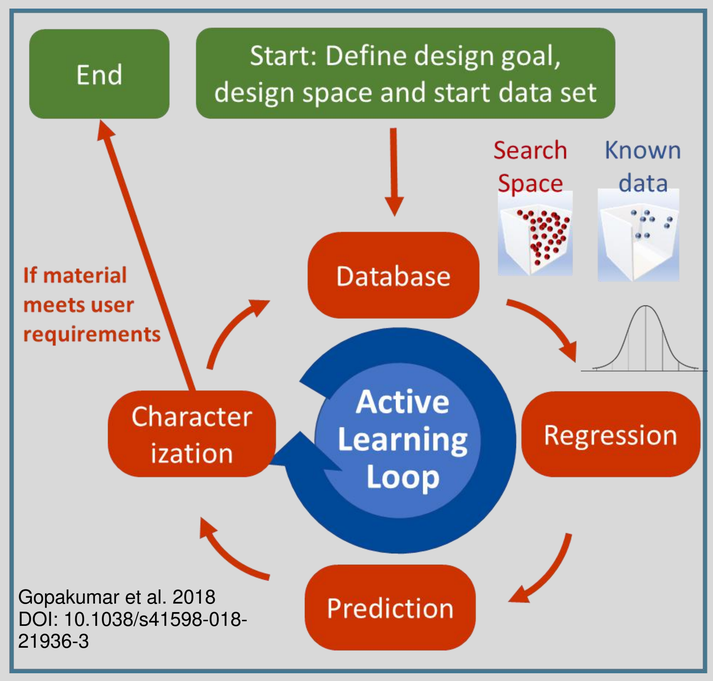
*Framework for **physics based modeling and Bayesian optimization***

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.

Acknowledgement:

COMET program within the K2 Center "Integrated Computational Material, Process and Product Engineering (IC-MPPE)" (Project No 859480). This program is supported by the Austrian Federal Ministries for Climate Action, Environment, Energy, Mobility, Innovation and Technology (BMK) and for Digital and Economic Affairs (BMDW), represented by the Austrian research funding association (FFG), and the federal states of Styria, Upper Austria and Tyrol.

MATERIALS CENTER LEOBEN FORSCHUNG GMBH