

Topic for a Bachelor Thesis

Database Development for Storage of Computational and Experimental Data

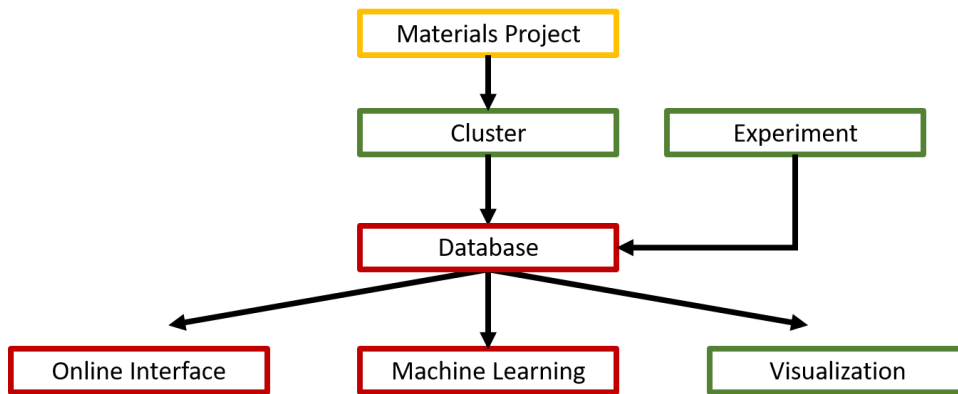


Fig 1: Schematic Overview

The target of this thesis is to construct a SQL-database that stores the computational and experimental results of the 1. Institute of Physics.

These results include among others optical data (Dielectric Function), band

structures, Density of States (DOS), effective mass tensors and quantum-chemical descriptors like the number of Electrons Shared (ES) and Transferred (ET).

Currently, data for around 1000 compounds are available. An easy and structured access to the values would enable the usage of the results for Machine Learning applications, which could be a consecutive addition to this thesis, i.e. inferring from the band structure to ES/ET values. Fig 1. depicts the database as the center piece of the workflow, as all results are collected within it, and then distributes the results to other application like an online interface for searching the database, as well as visual representation.

The main task of the thesis is to develop the database and fill it with the data already available, i.e. writing a script to do automate this task.

Requirements: The student should have moderate coding experience and be interested in independent problem solving. Prior knowledge of SQL and Machine Learning is beneficial, but not required.