Computational Materials Database

About

This document describes the concept and the proposed development process for a computational materials database. The database serves as the primary hub to import and export simulation data of materials simulations.

For early tests the database is exclusively used by the Glotzer Group at the University of Michigan. Later stages may provide (general) public access.

Development Process

Development Stages

1. Basic Design / Requirements
    a) Concept for technical framework
    b) Concept for standard models
    c) Test of alpha features
2. Detailed Design / Early Implementation
    a) Revision of technical framework
    b) Revision of standard models
3. Implementation
4. Testing

Milestones

1. Define technical framework.
2. Define internal standard for model representation.
3. Provide testing data.
4. Implement alpha requirements.
    - Import structures from local files
    - Export structures to local files
    - Import structures for simulation runs
    - Export structures from simulation runs
5. Implement beta requirements.
    - View files in browser
    - Import and export force field setup
    - Import and export job script
    - Generate pair potential from DB

Technical Description

Use cases

- Import structures from simulation data
- Import structures from other databases
- Export structures for analysis
- Export structures for simulation
- View structures online
- View analysis data online
- Apply analytical methods on database entries directly

Features

- All structures associated with citation info.
- Structures can be associated with simulation data.
- Structures can be associated with simulation job descriptions
- Auto-fetch of results, where results are available.

Supported Formats

Structures are translated via an internal python class (IPC), which serves as intermediate layer to translate between formats.

For import:

- HoomdXML
- CIF
- libgtar
- PDB

For export:

- HoomdXML
- CIF
- numpy arrays

Supporting tools

- django
- MongoDB
- JMol
- injavis