Python Materials Discovery Framework (PyChemia)

WEB REPORTING
Visualization
Tables and plots

DATABASE
MongoDB
NoSQL database

METADATA
Structure tags and
Phylogenetic history

STRUCTURAL SEARCH

OPTIMIZATION

Minimal Hoping Method

Genetic Algorithms

Swarm Algorithms

Neural Networks

...

DATA MINING

Anomaly Detection

Association Rules

Clustering

Classification

Regression

Summarization

ANALYSIS
Band Structures
Density of States
Electron locality
Properties:
    Mechanical
    Optical
Symmetry
Similarity
Phonons
Thermal stability

PyChemia Structure Object

Utils
(Physical constants,
Periodic Table)

FILE FORMATS AND OBJECTS

JSON Serialized
Structure

VASP
POSCAR

ABINIT
abinit.in

CIF

OpenBabel

External Objects
PYMATGEN
ASE