Python Materials Discovery Framework (pyQuimia)

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

pyQuimia 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