Workflow for Python Materials Discovery Framework (pyQuimia)

KNOWN STRUCTURES From experimentally synthetized or theoretically predicted STRUCTU

NEW STRUCTURES

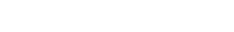
New potential structures are produced



SIMILARITY ANALYSIS

Compared with structures already in the database.
Structural fingerprints

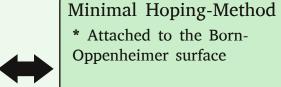




STRUCTURAL SEARCH

Genetic Algorithms

* More random
exploration



Constraints

Coordination, symmetry, local structures, physical properties









Density-Functional Theory and Tight-Binding codes

VASP

ABINIT

Fireball

DFTB+

STABILITY ANALYSIS

Chemical Stability (Enthalpy) Dynamical Stability (Phonons)



DATABASE

Structure, phylogenetic history and properties are stored



WEB INTERFACE

Visualization Tables and plots