Workflow for Python Materials Discovery Framework (PyChemia)

KNOWN STRUCTURES
From experimentally synthetized or theoretically predicted

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

Minimal Hoping-Method
* Attached to the Born-Oppenheimer surface

Constraints
Coordination, symmetry, local structures, physical properties

STABILITY ANALYSIS
Chemical Stability (Enthalpy)
Dynamical Stability (Phonons)

DATABASE
Structure, phylogenetic history and properties are stored

Density-Functional Theory and Tight-Binding codes

VASP   **ABINIT**   **Fireball**   **DFTB+**

WEB INTERFACE
Visualization
Tables and plots