PyChemia: Software Package for High-Throughput Materials Discovery

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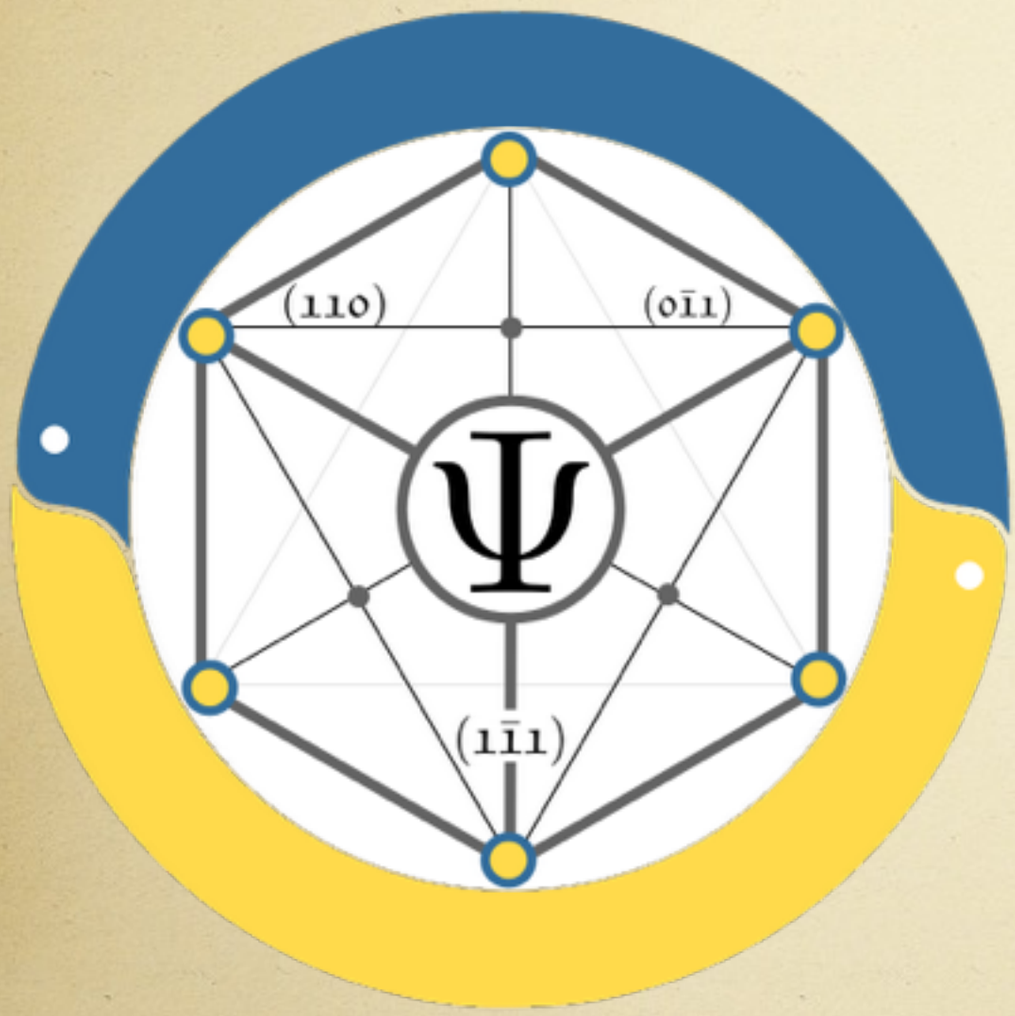
What is PyChemia?

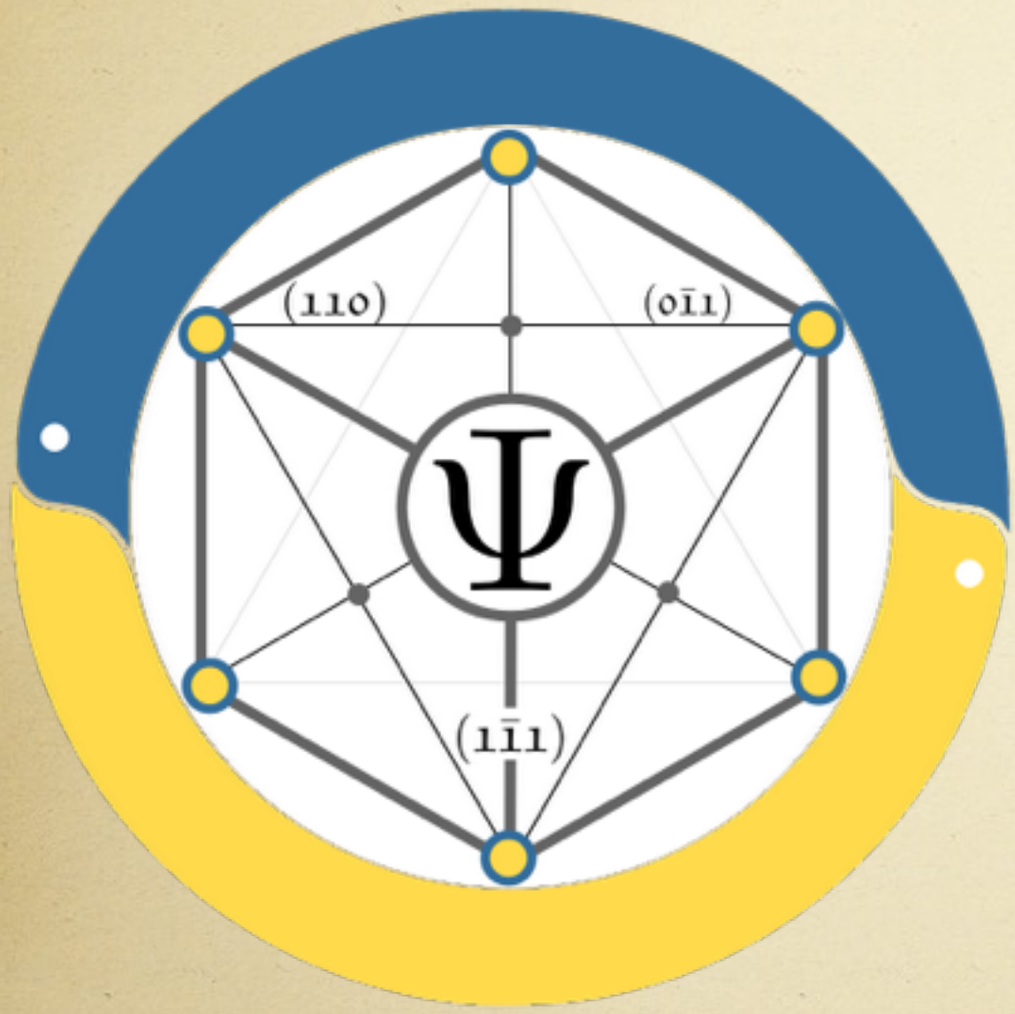


GitHub

PyChemia is an open-source Python Library

https://github.com/MaterialsDiscovery/PyChemia

What is PyChemia?



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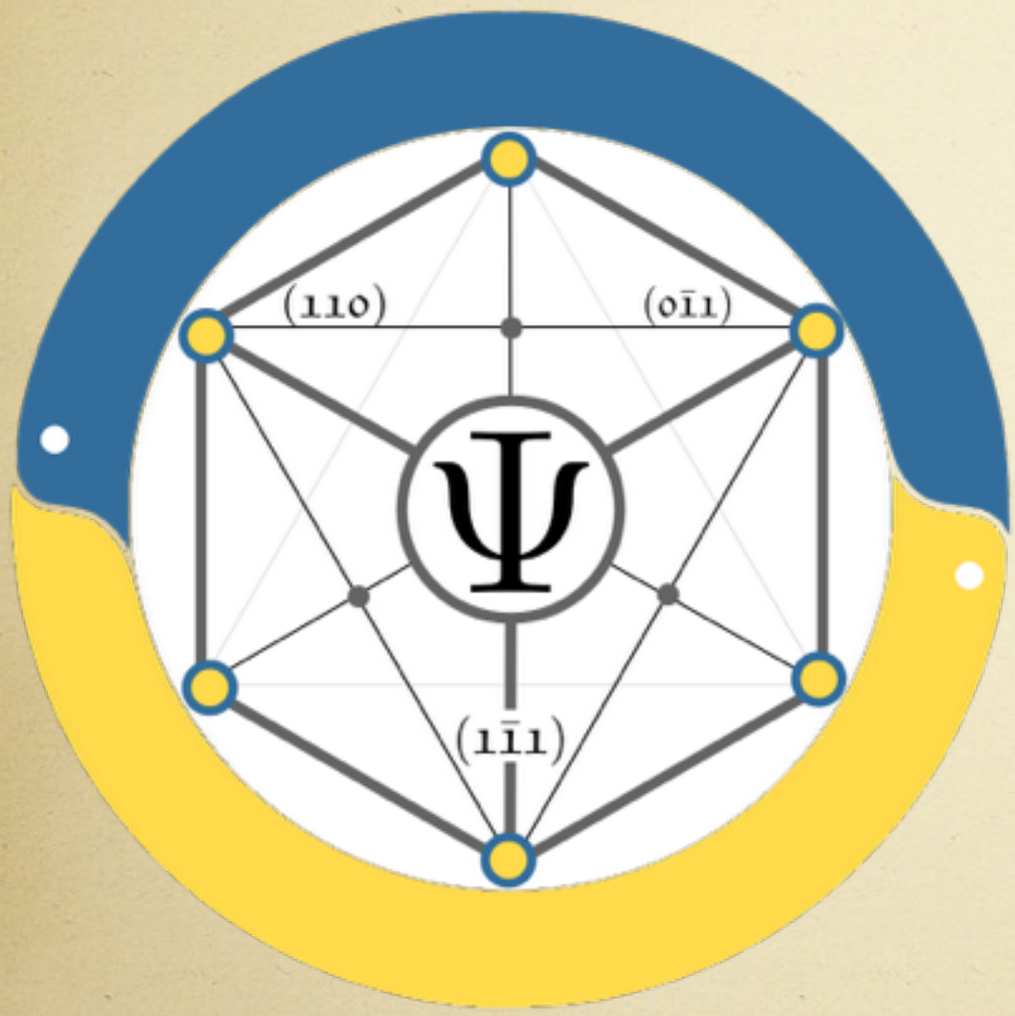
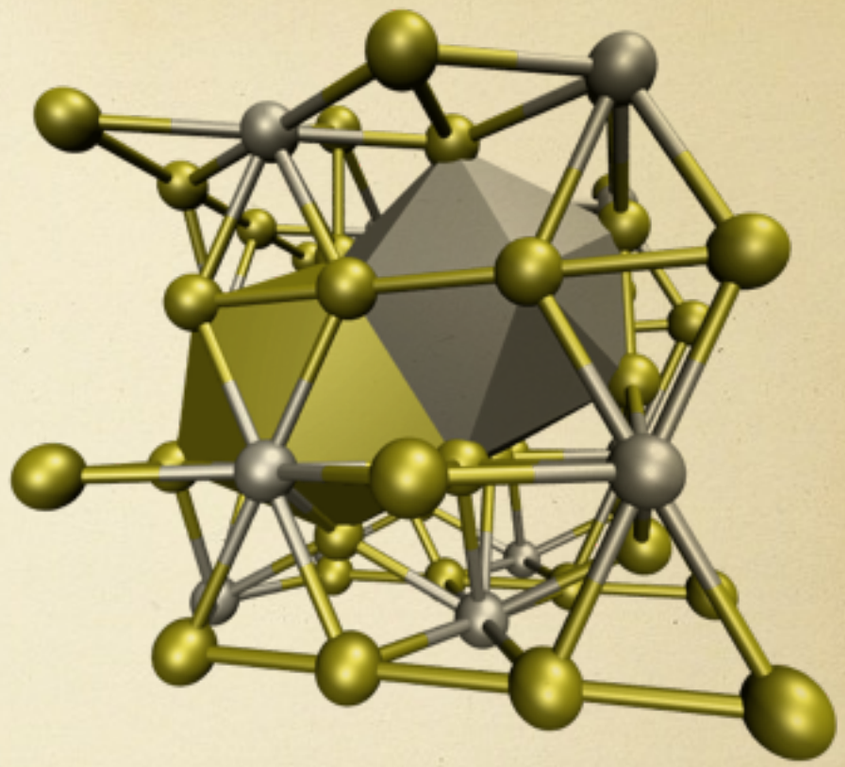
Interfaces with atomistic simulation packages

What is PyChemia?

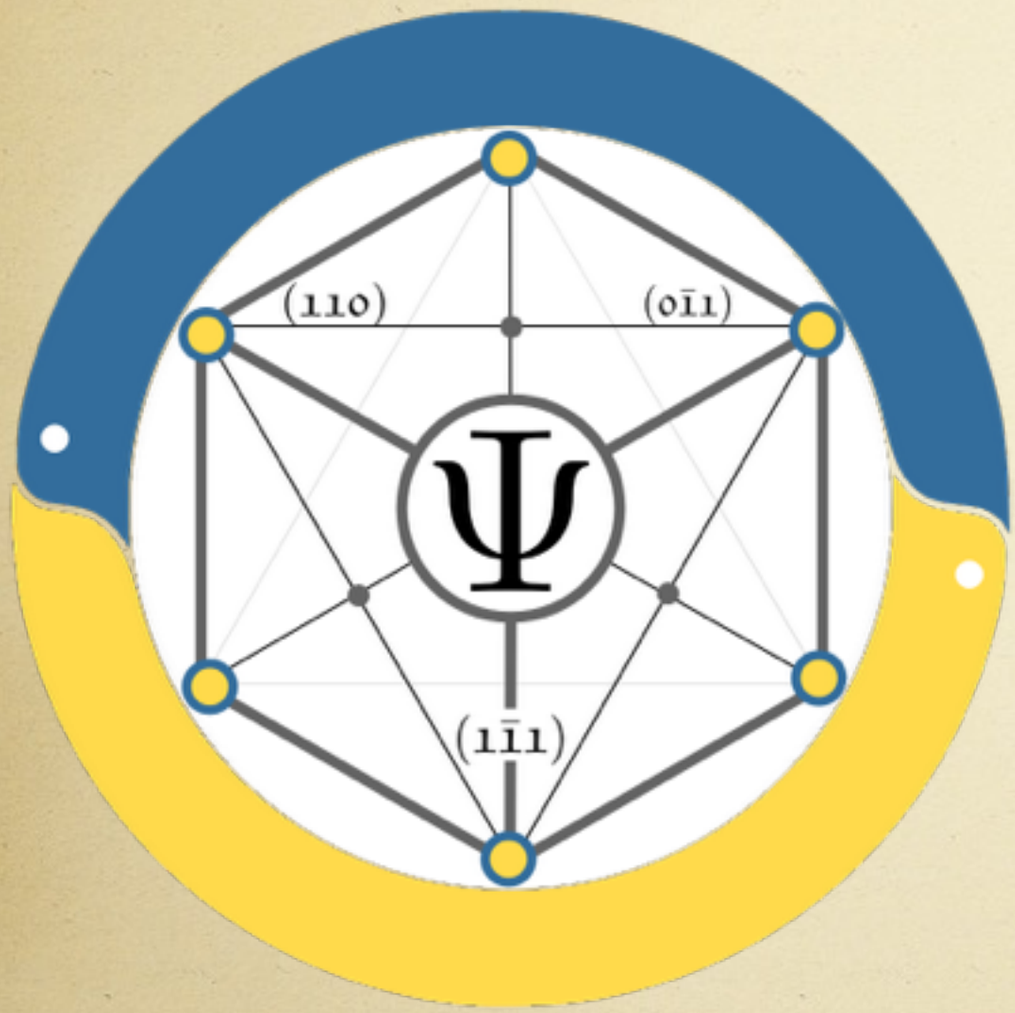




Static Calculations
Relaxation
Parameter Convergence
Ideal Strength
ElasticModuli
Polarization

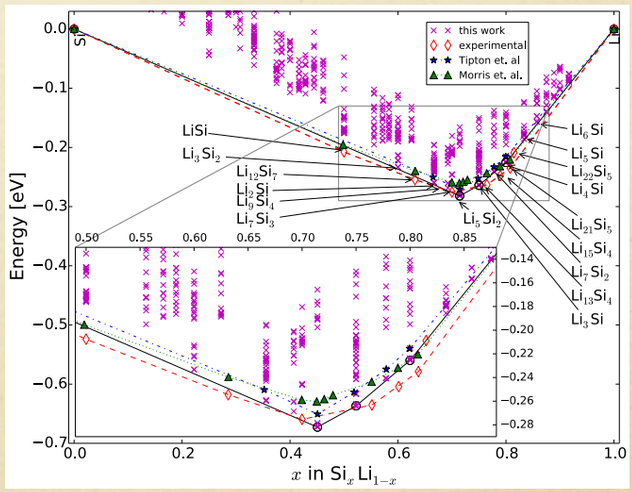
To automatize the execution of tasks

What is PyChemia?

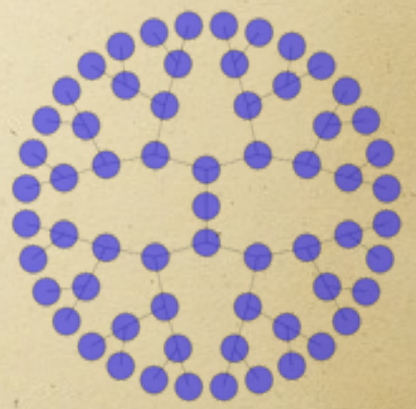


Metaheuristics

Convex Hulls



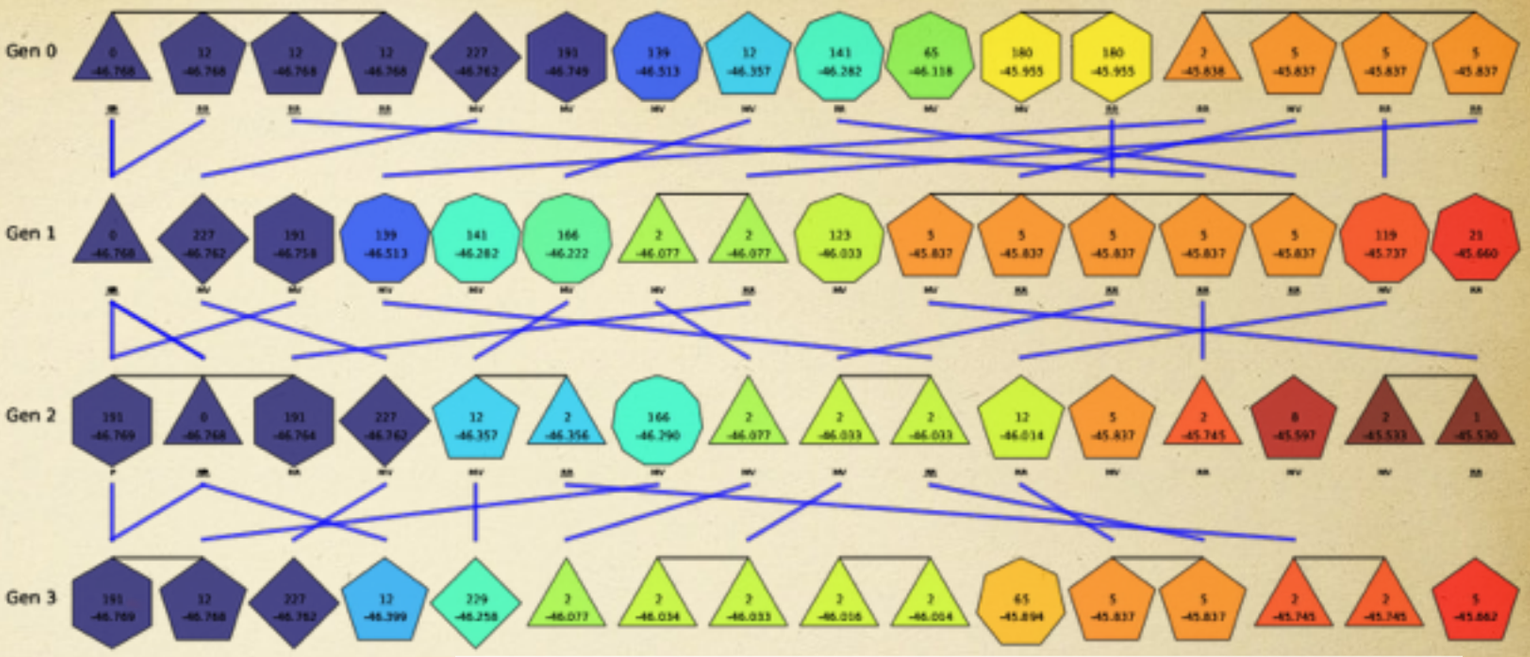
Tree Search

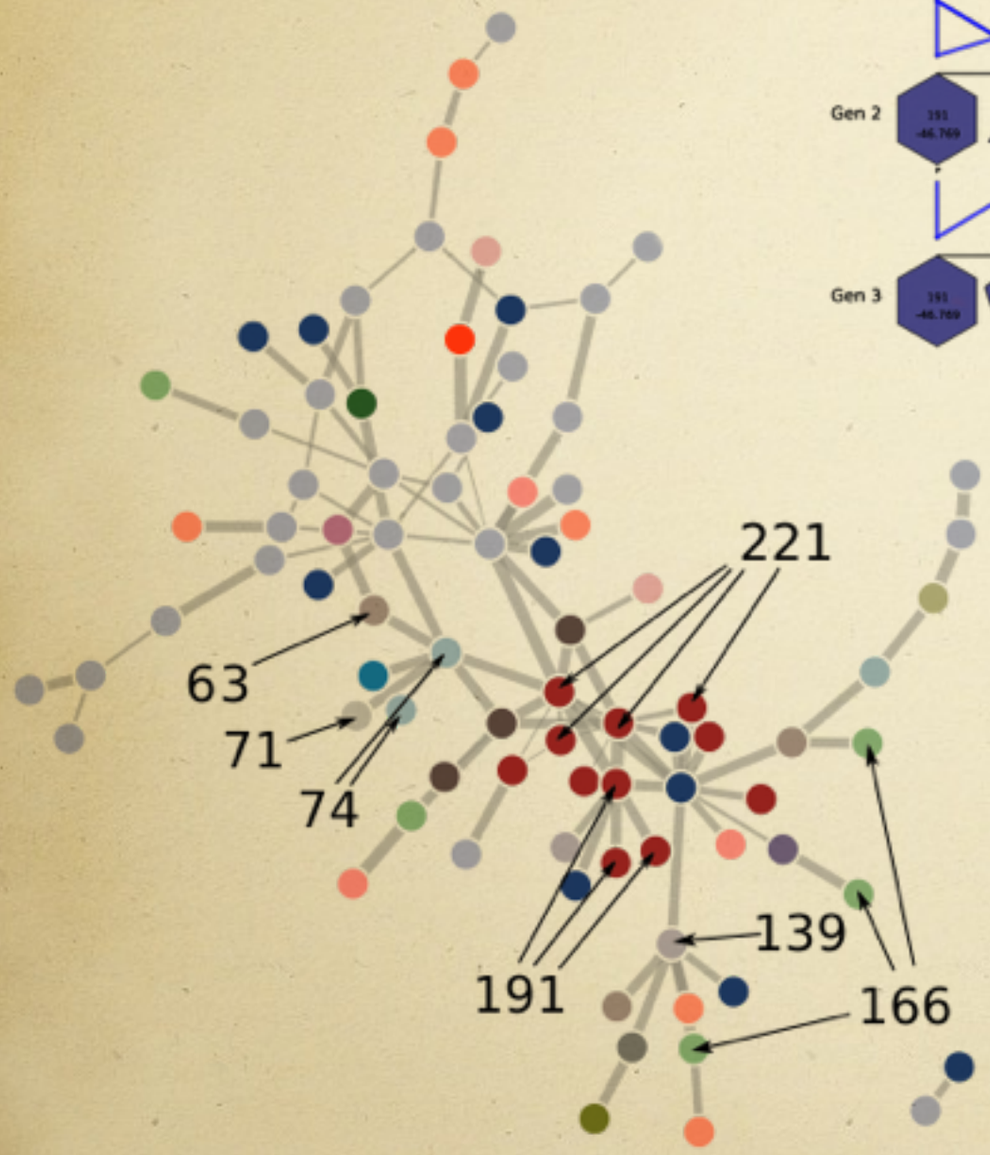


And more complex executions

mongoDB

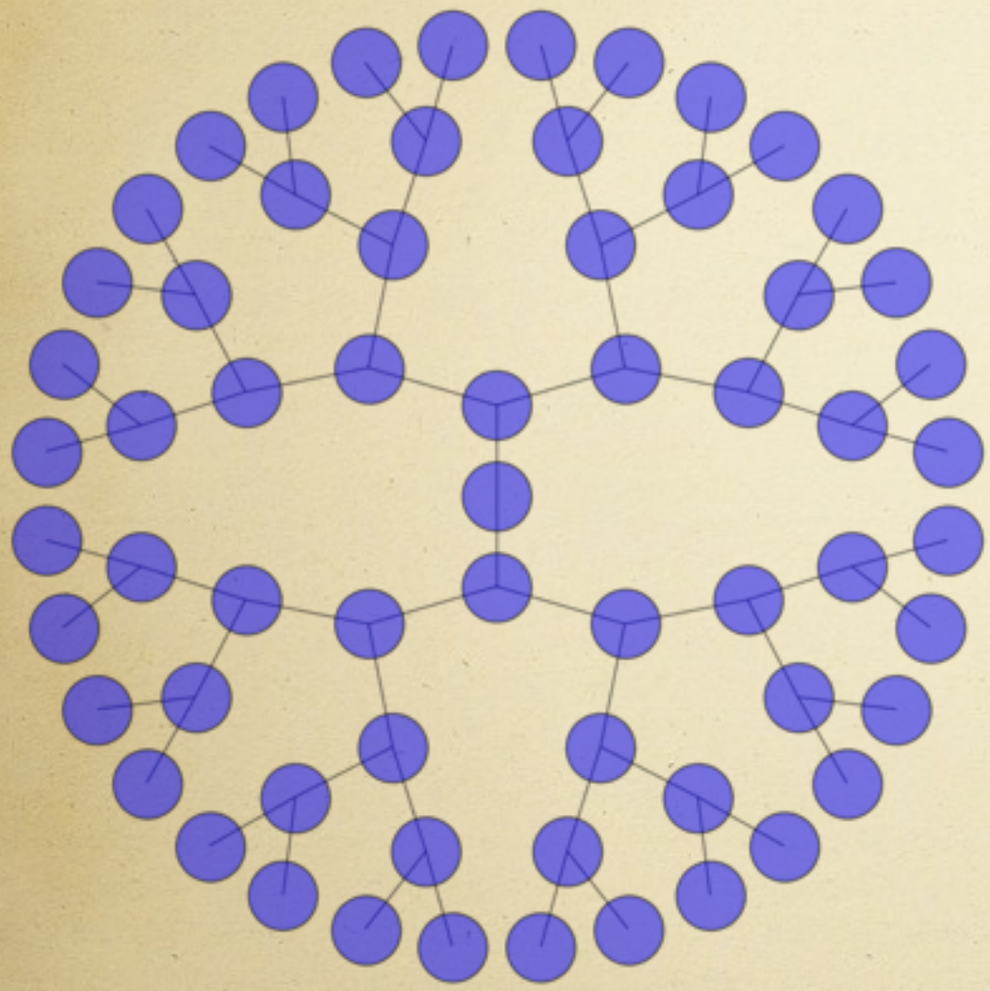
PyChemia

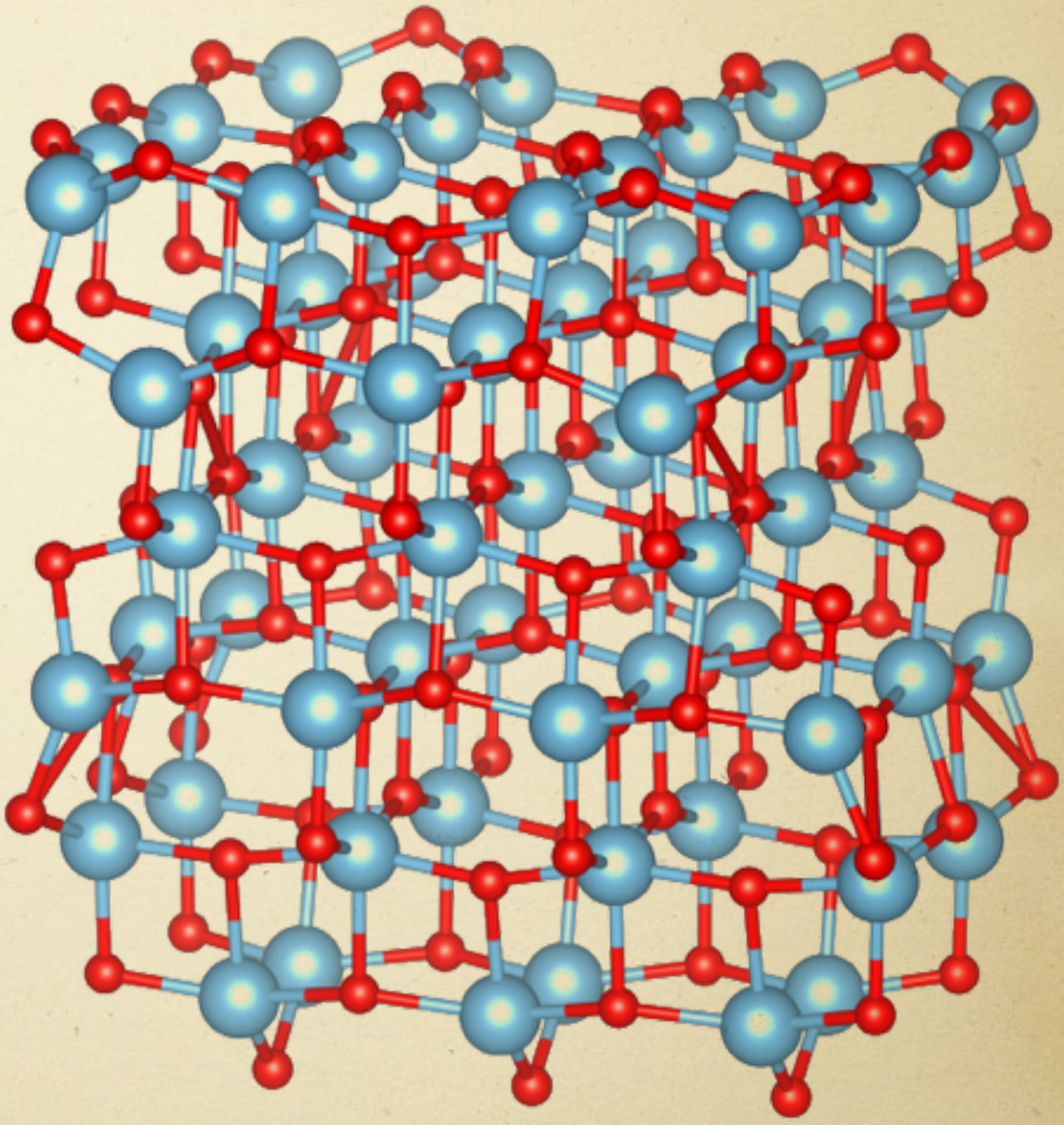




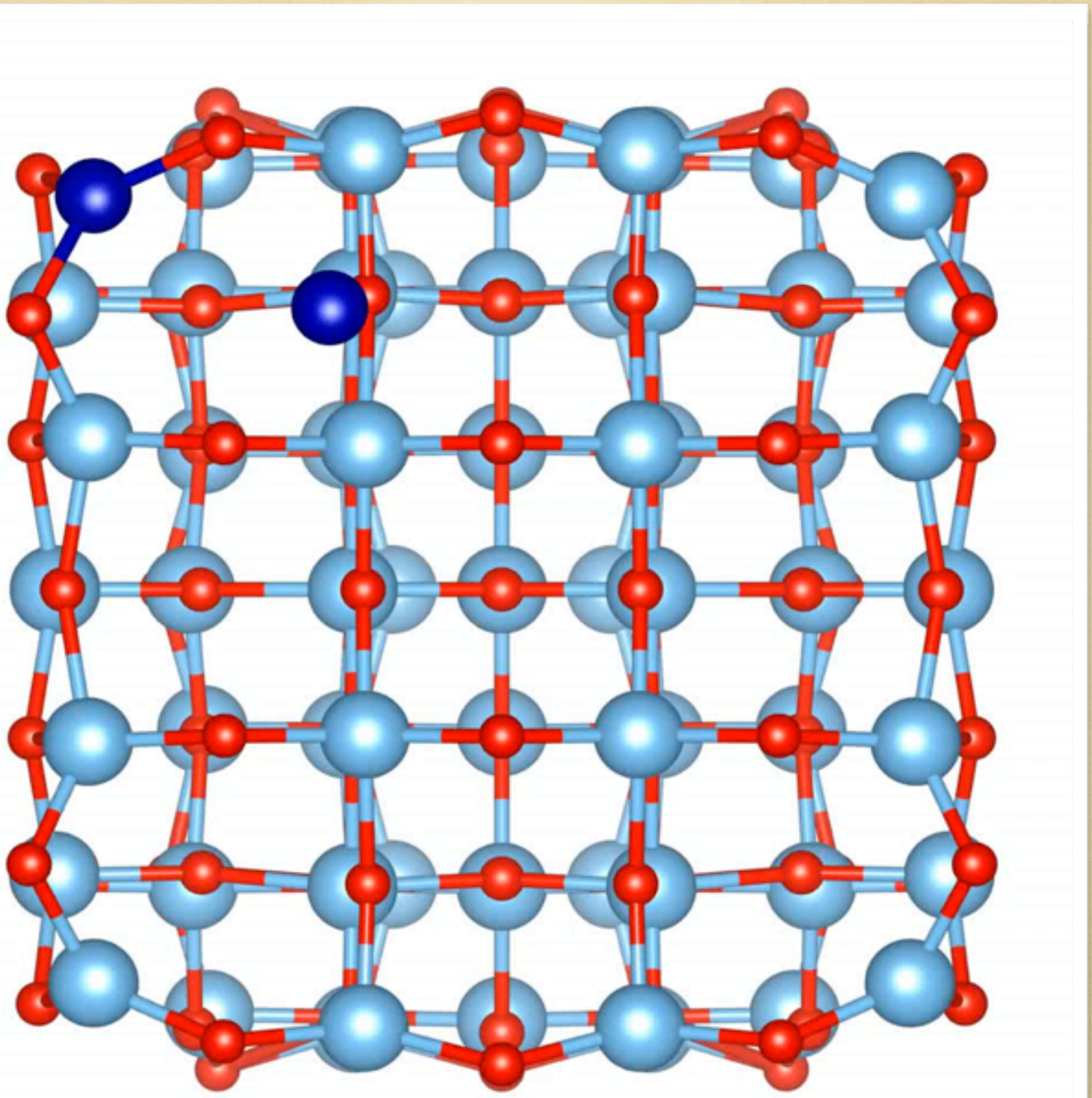
Analytics and Visualization

Applications: Tree Search

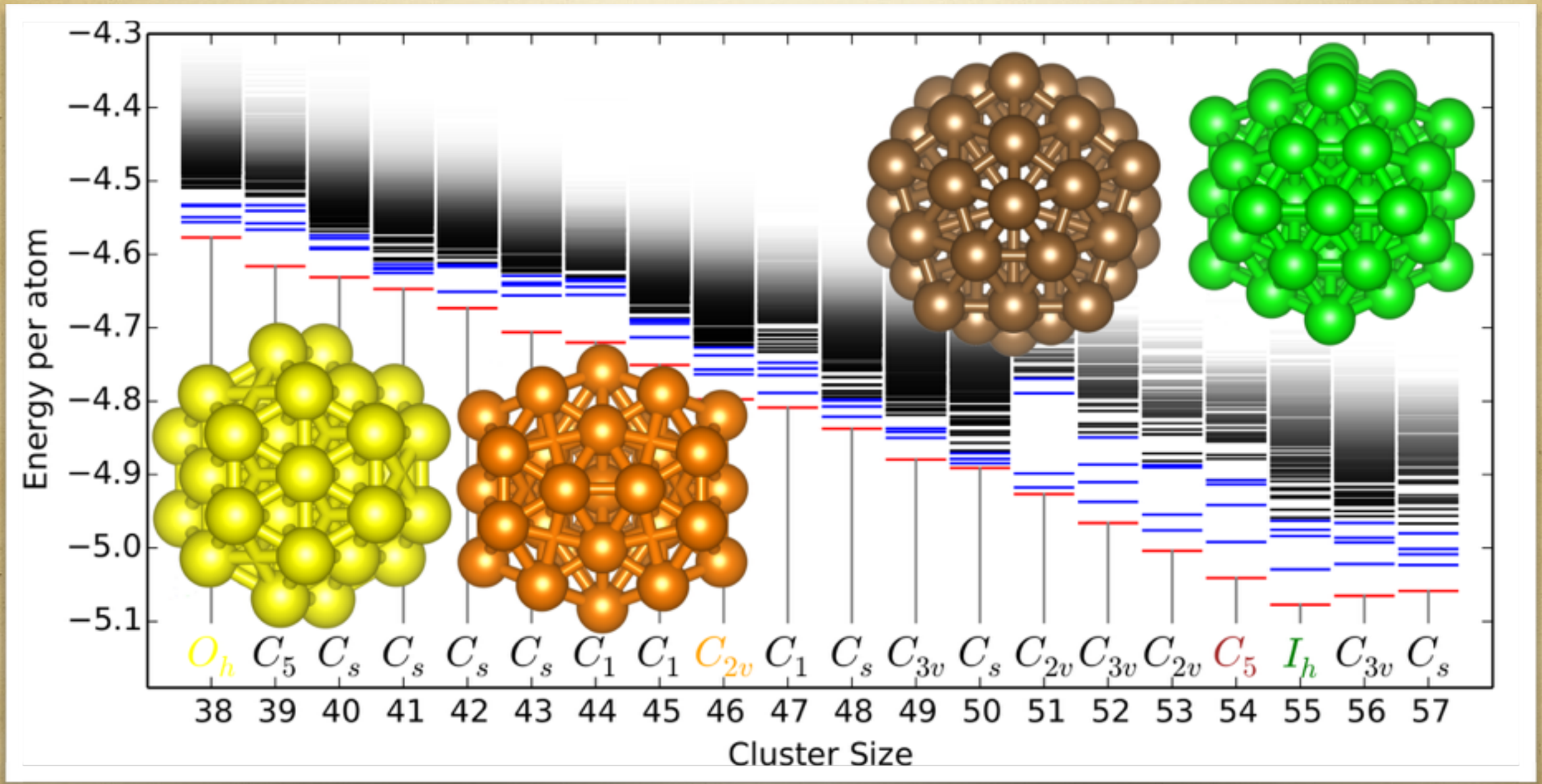


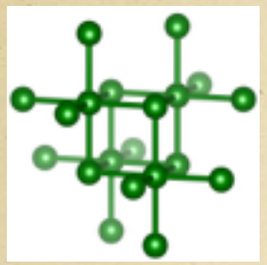


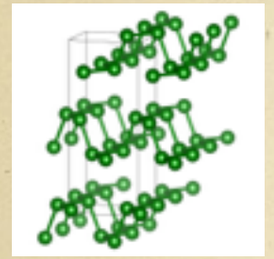
TiO_2

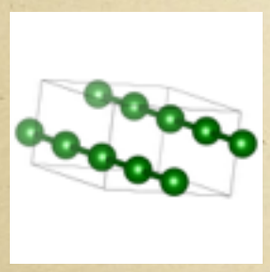


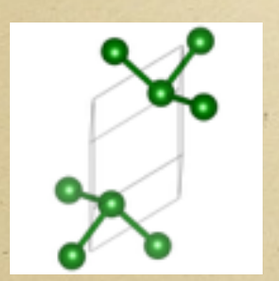
Metaheuristic Global Search: Lennard-Jones Clusters

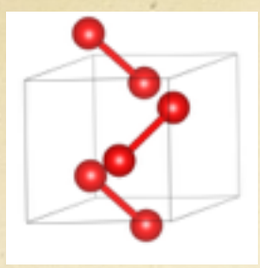


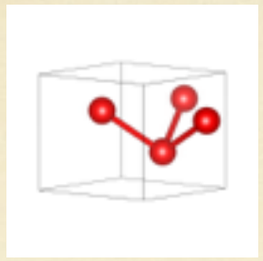


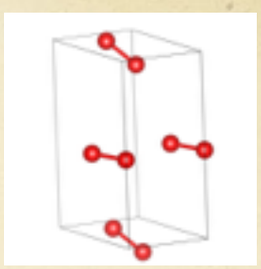


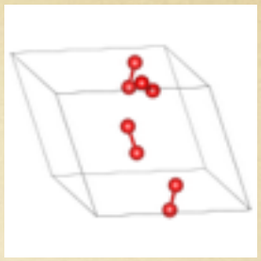


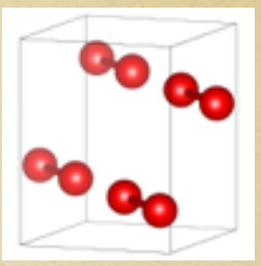


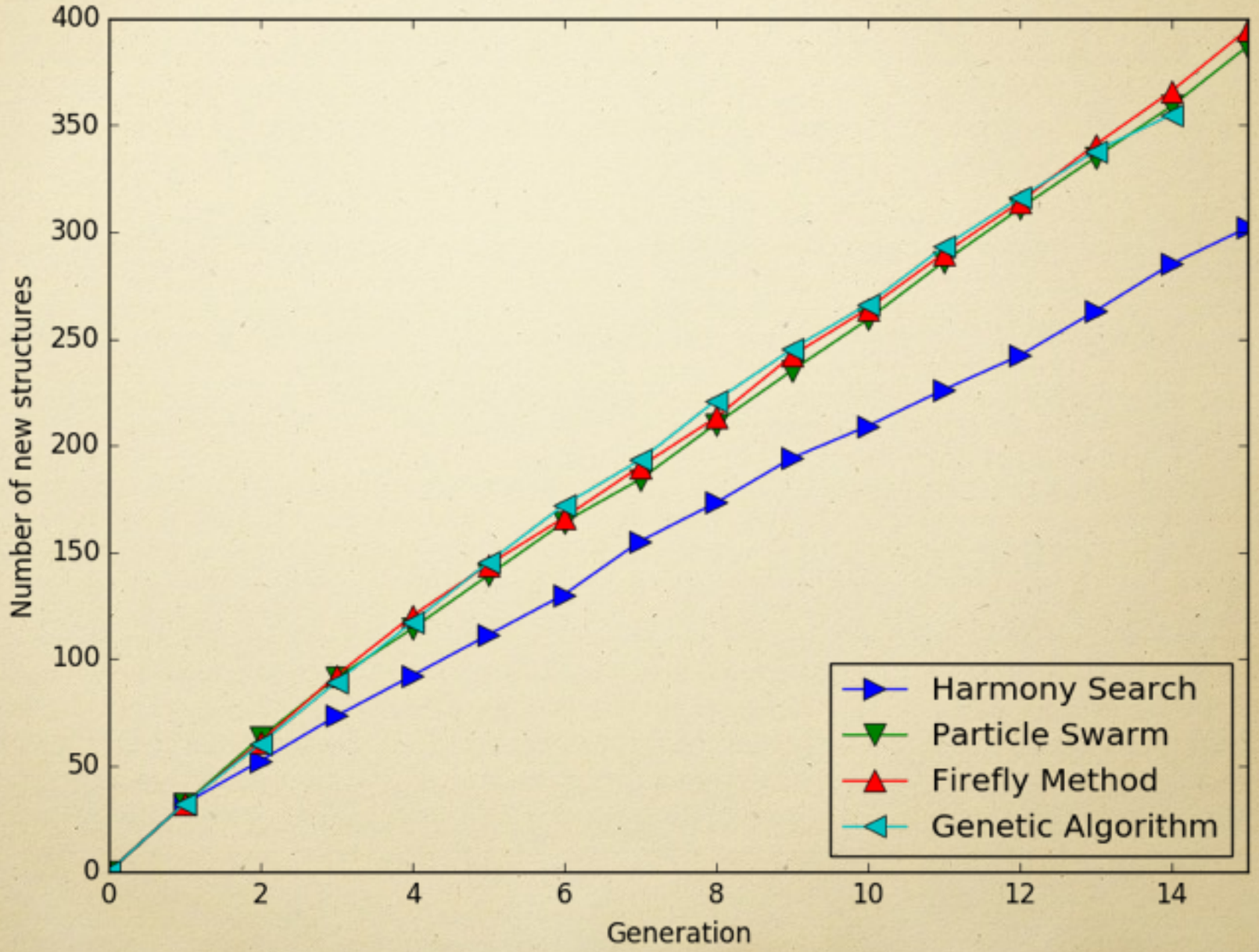








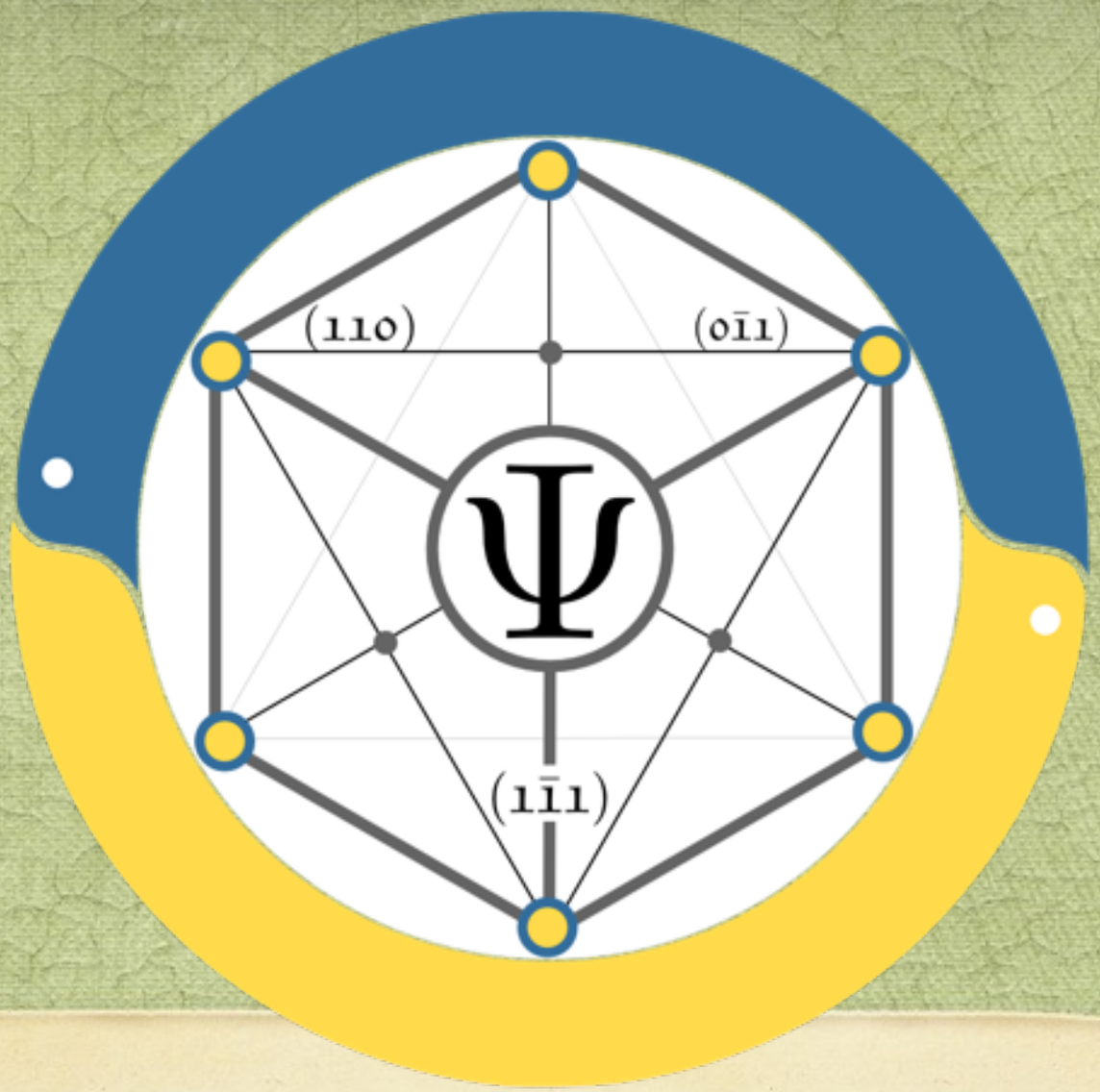




K23: Wednesday, March 16, 2016 10:24AM - 10:36AM

Conclusions

- We present PyChemia an open-source python library for High-Throughput Materials Discovery.
- We show a variety of applications where PyChemia has been applied.
- Invited to K23: Wednesday, March 16, 2016 10:24AM - 10:36AM about a new metaheuristic method implemented on PyChemia



Thank You

gufranco@mail.wvu.edu

https://github.com/MaterialsDiscovery/PyChemia