

Computational Discovery of Materials Using the Firefly Algorithm

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Summary

- Present the implementation of the Firefly method applied to structural search of periodic and non-periodic systems
- Apply the method to Lennard-Jones Clusters and Phosphorus crystals
- Describe how the Firefly method is integrated into PyChemia, an open source python library for manipulating, running, and analyzing atomic-level simulations.

Global Search Methods and Structural Search of Materials

Stochastic methods

Random Search

Basin hoping

Metaheuristics

Dynamic methods

(Minima Hoping)

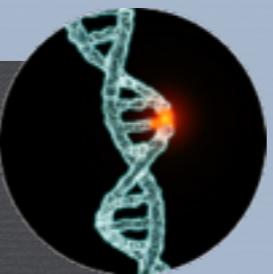
Data-mining
methods

Global Search Methods and Structural Search of Materials

Stochastic methods



Genetic Algorithms
Particle Swarm
Harmony Search
Bee Algorithm
Firefly method



Random Search

Basin Hoping

Dynamic methods

Data-mining methods

The firefly algorithm mimics the behavior of fireflies in nature



The movement of fireflies is modeled as

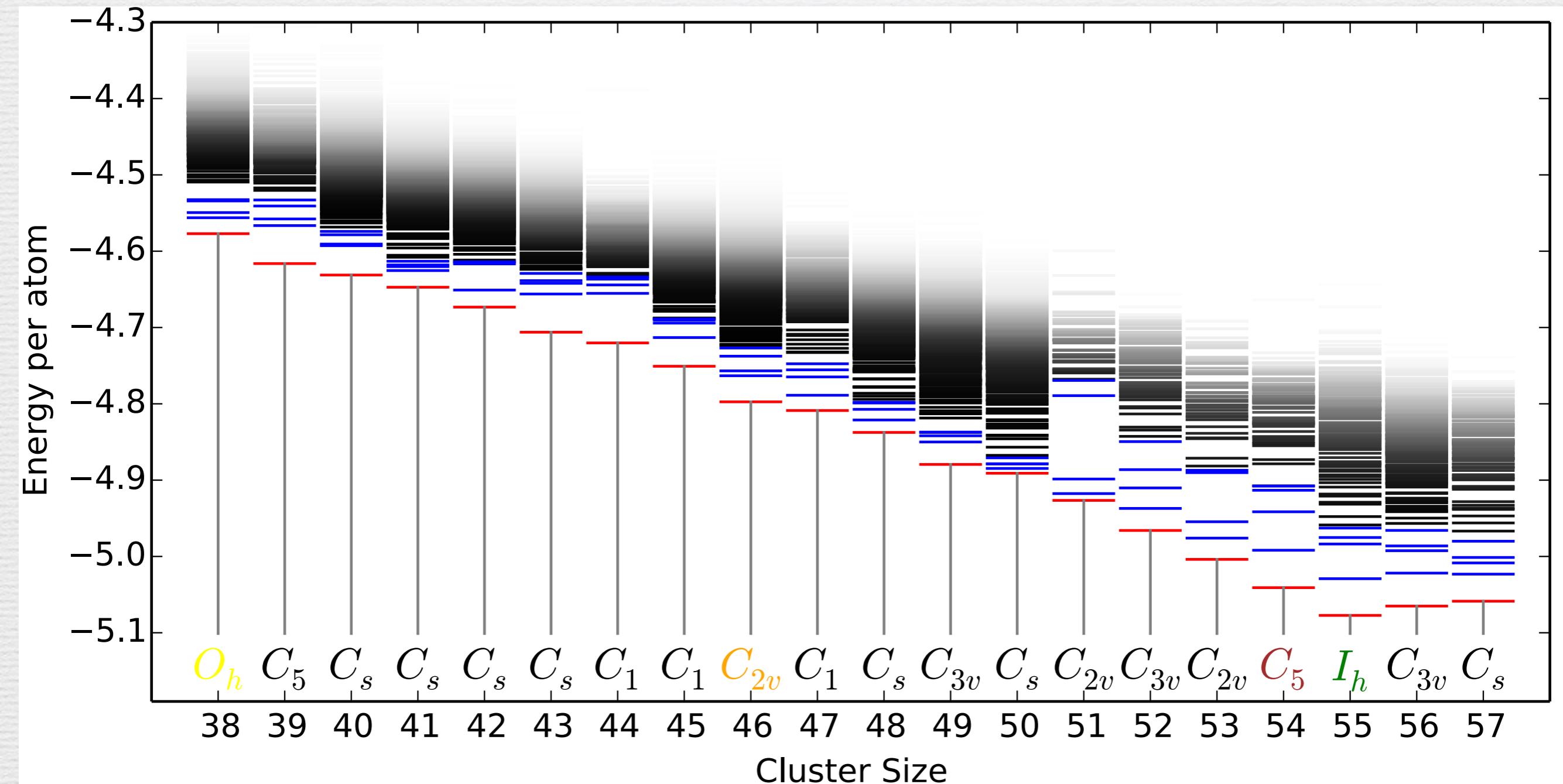
$$\mathbf{x}_i^{t+1} = \mathbf{x}_i^t + \sum_j \beta_0 e^{-\gamma r_{i,j}^2} (\mathbf{x}_j^t - \mathbf{x}_i^t) + \alpha^t \epsilon_i^t$$

- Intensity (Energy or Enthalpy)
- Distance (Fingerprint distance, Pair correlation function)
- Movement (Parametrization from structure A to B on configuration space)

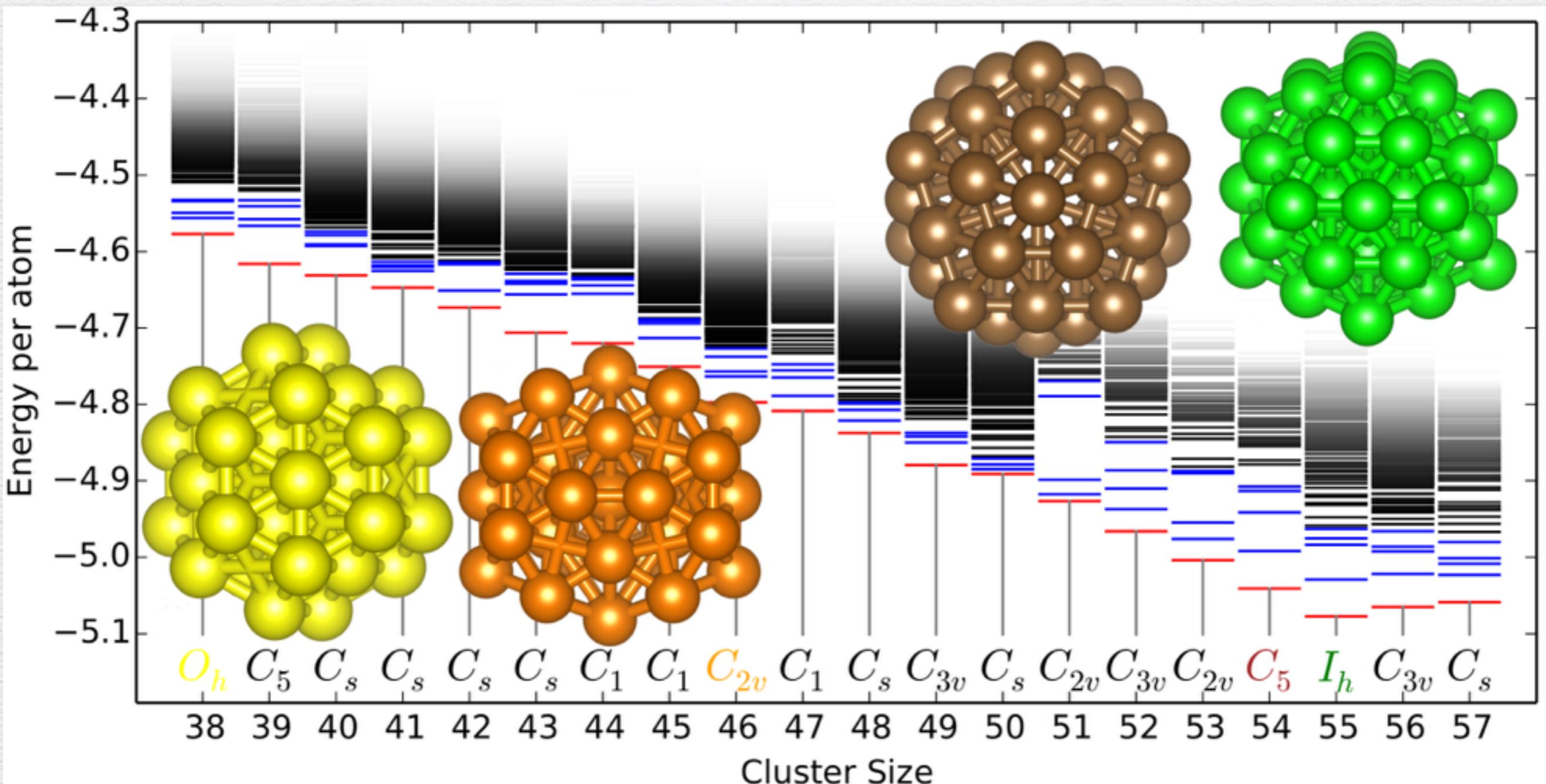


Finite Systems: Lennard-Jones Clusters

Lennard-Jones Clusters

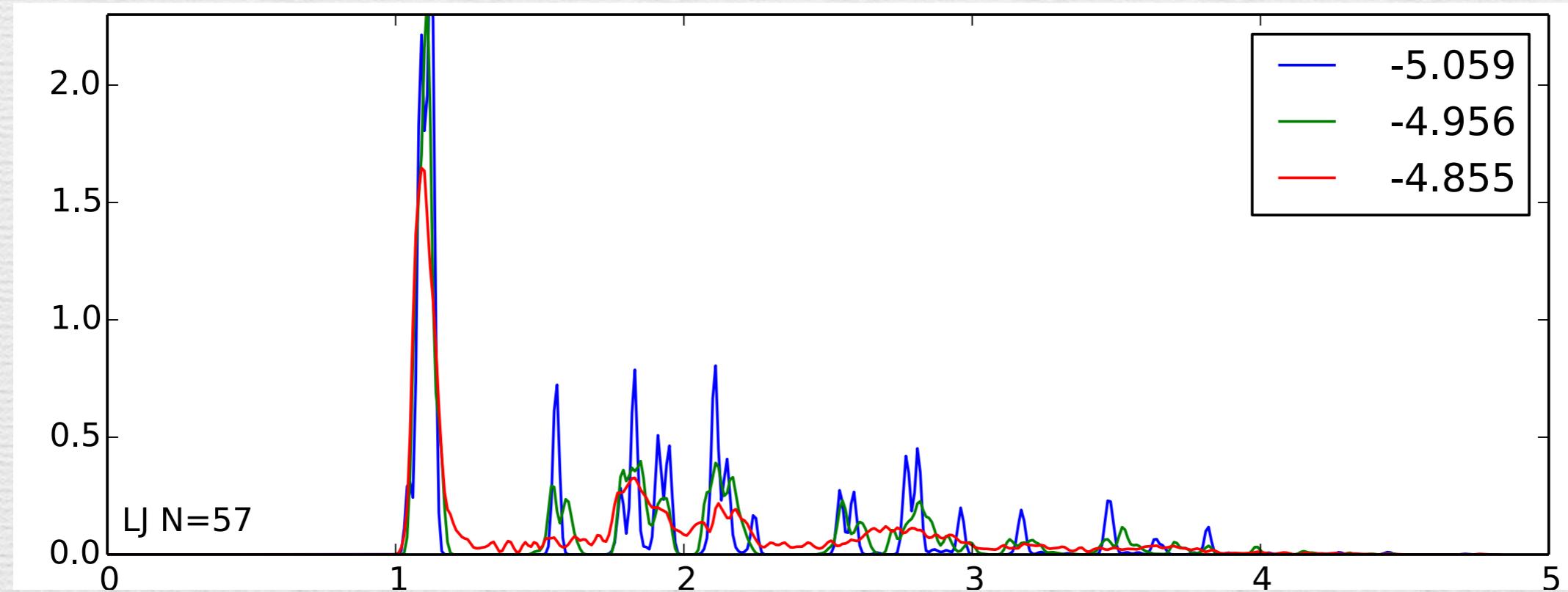
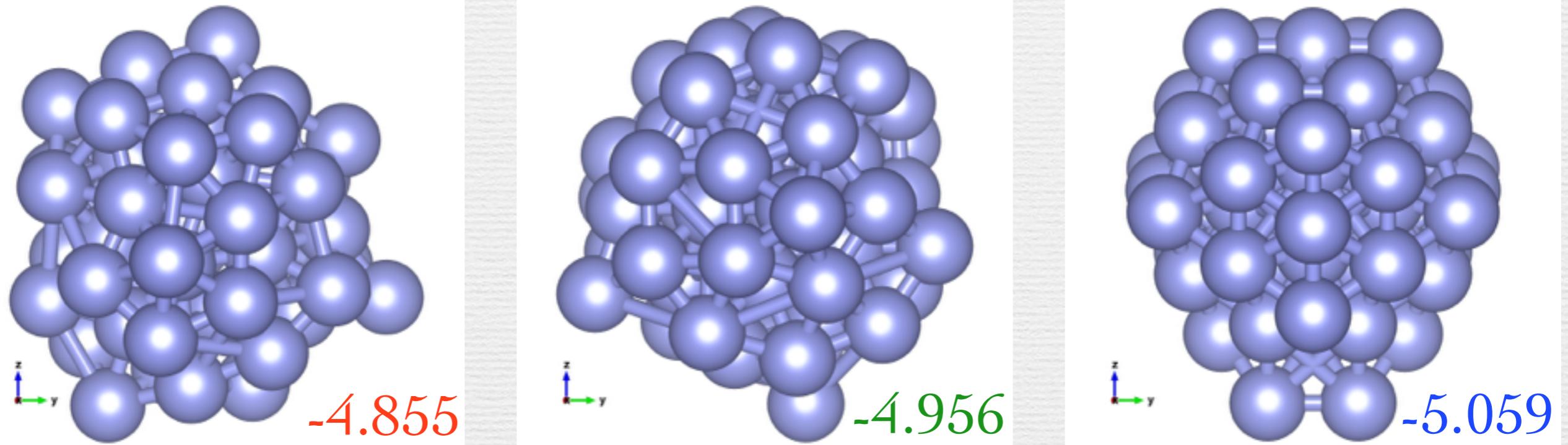


Lennard-Jones Clusters

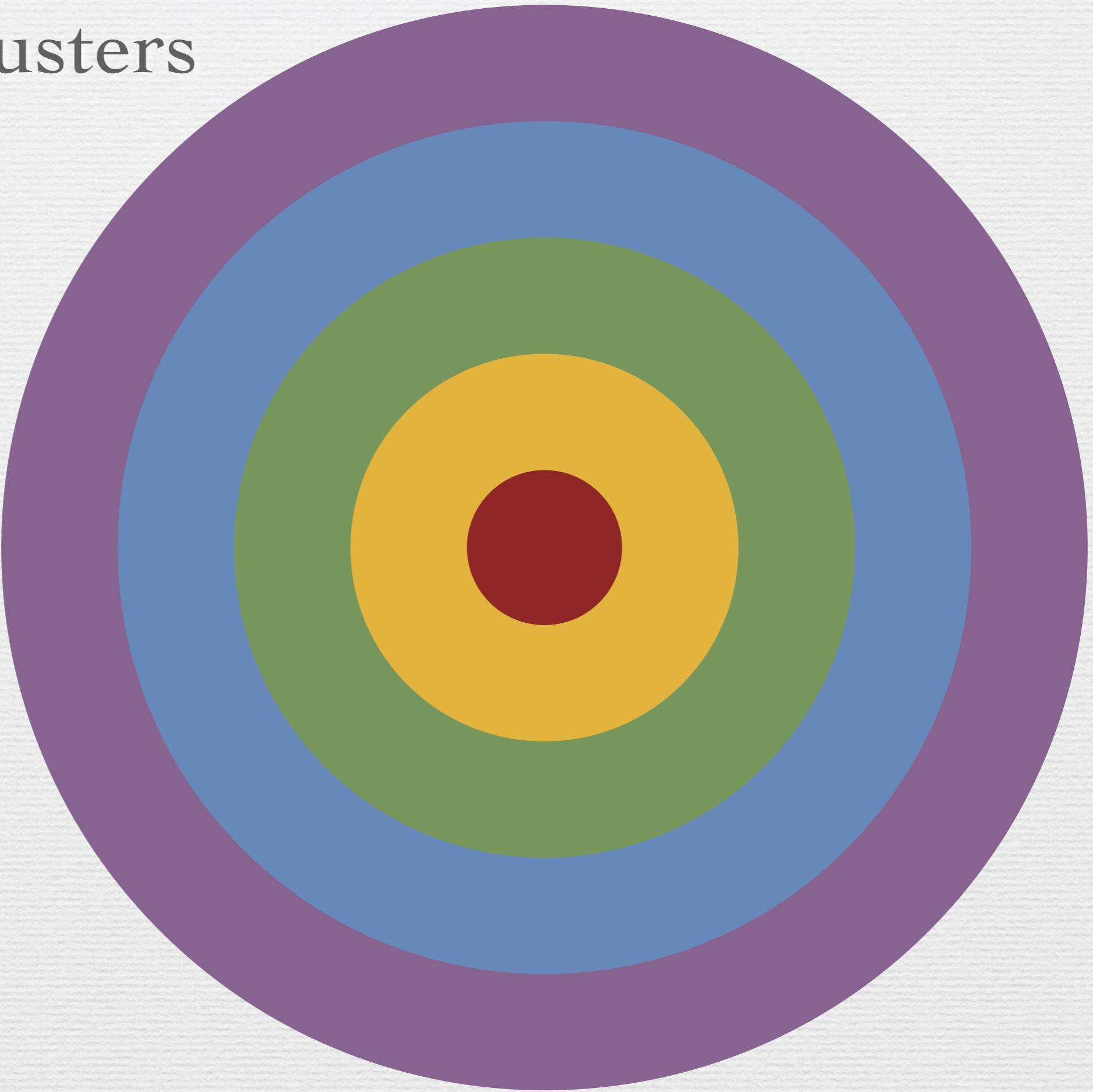


<http://doye.chem.ox.ac.uk/jon/structures/LJ.html>

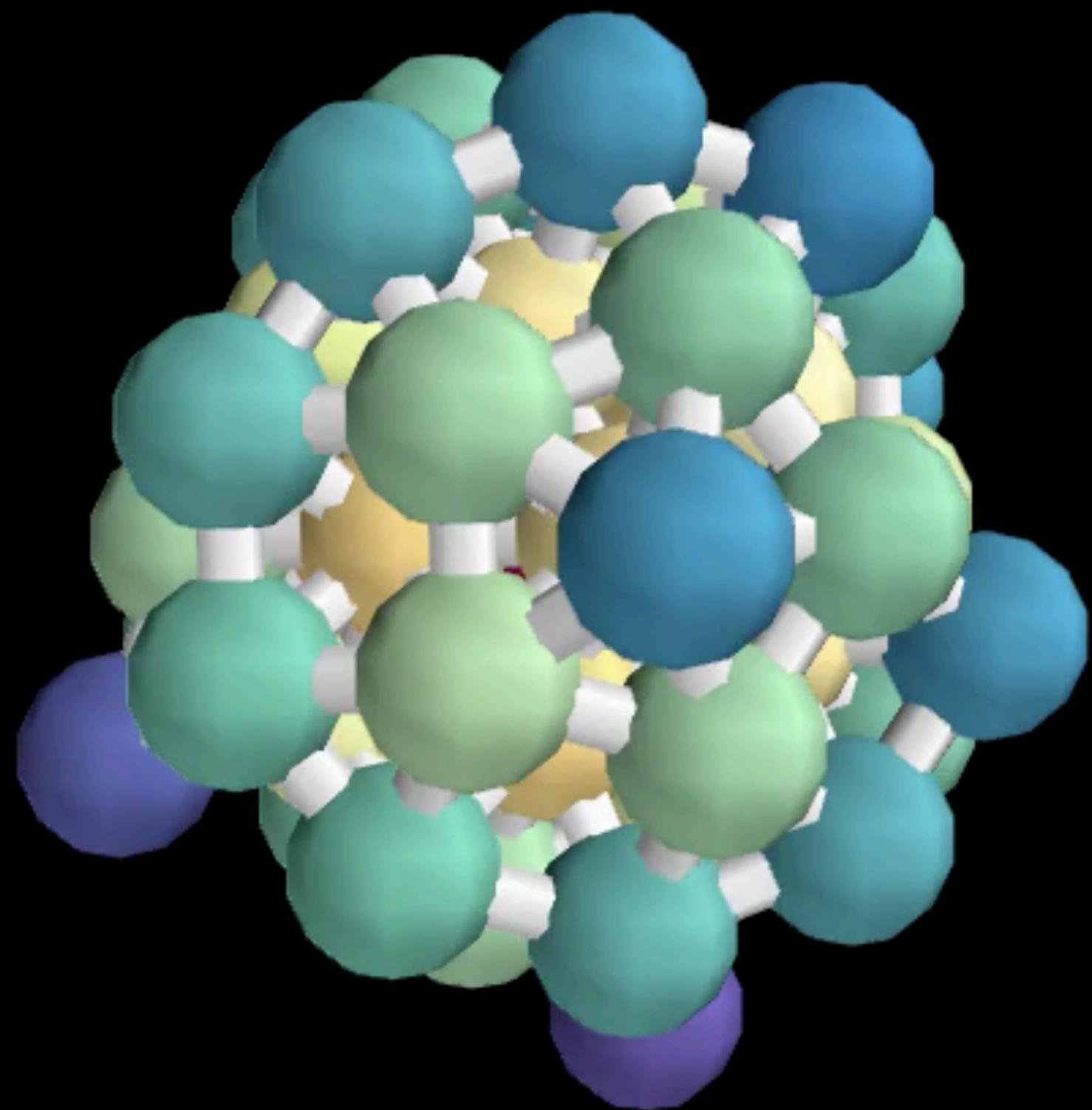
Lennard-Jones Clusters



Moving clusters

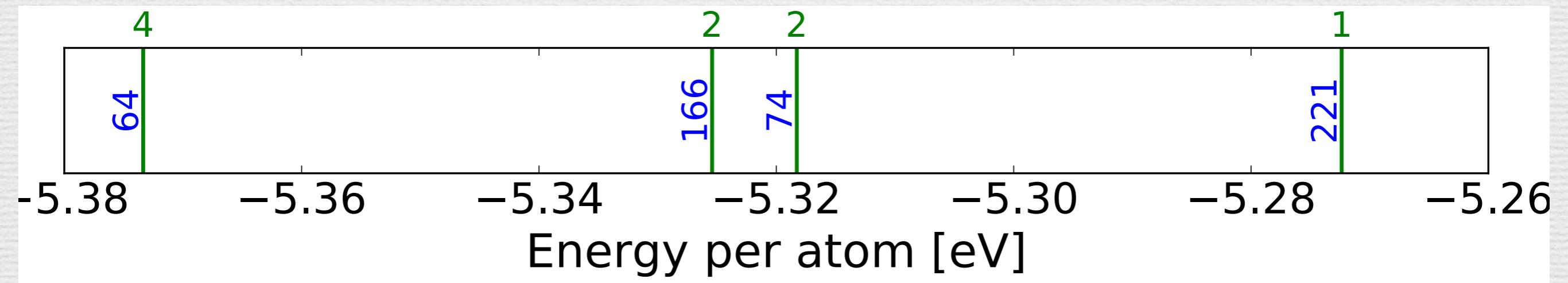
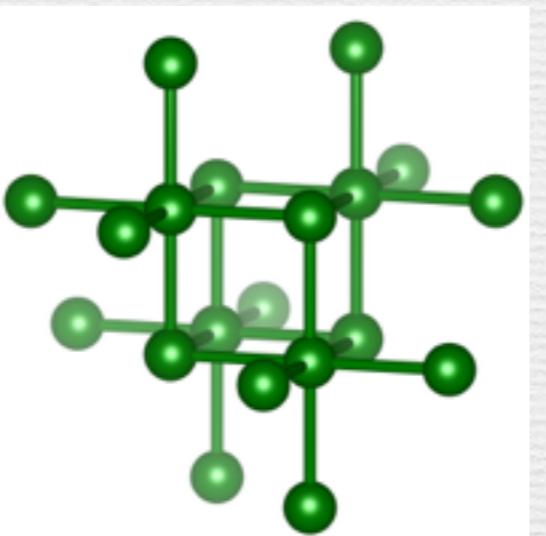
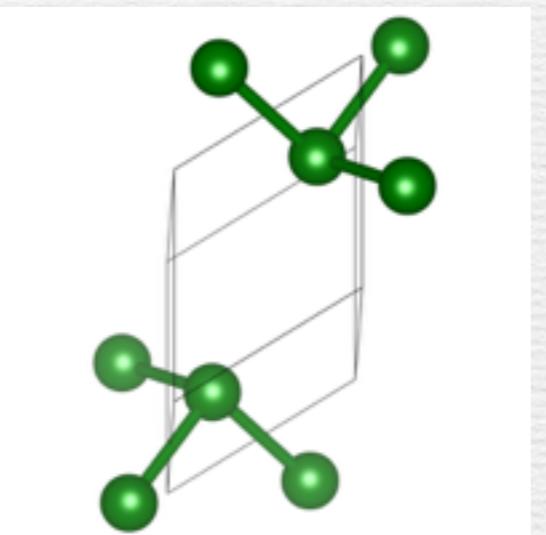
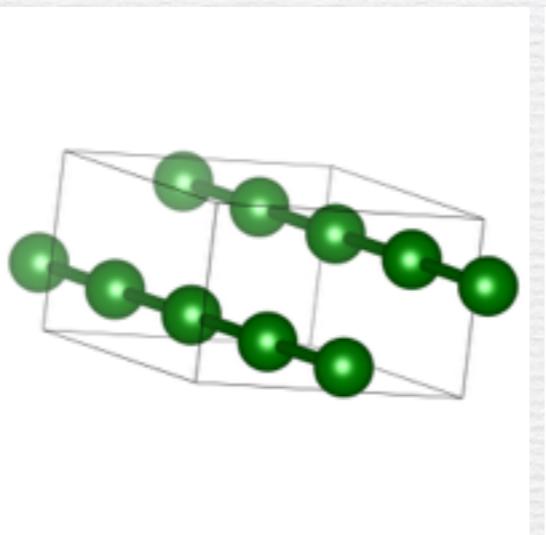
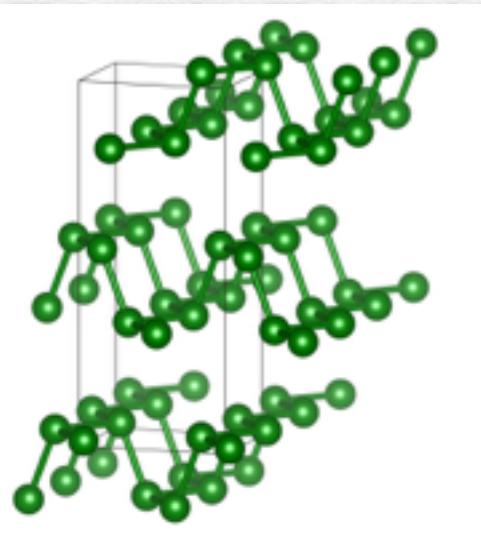


Lennard-Jones Clusters

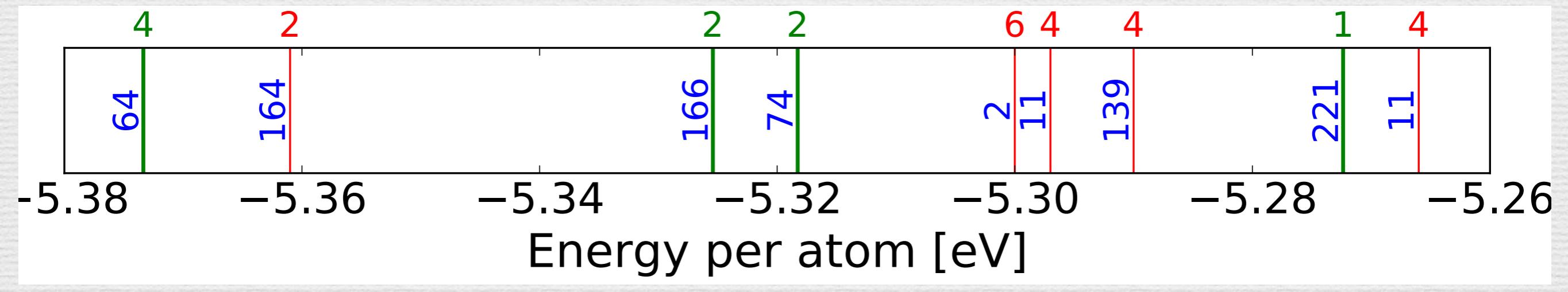
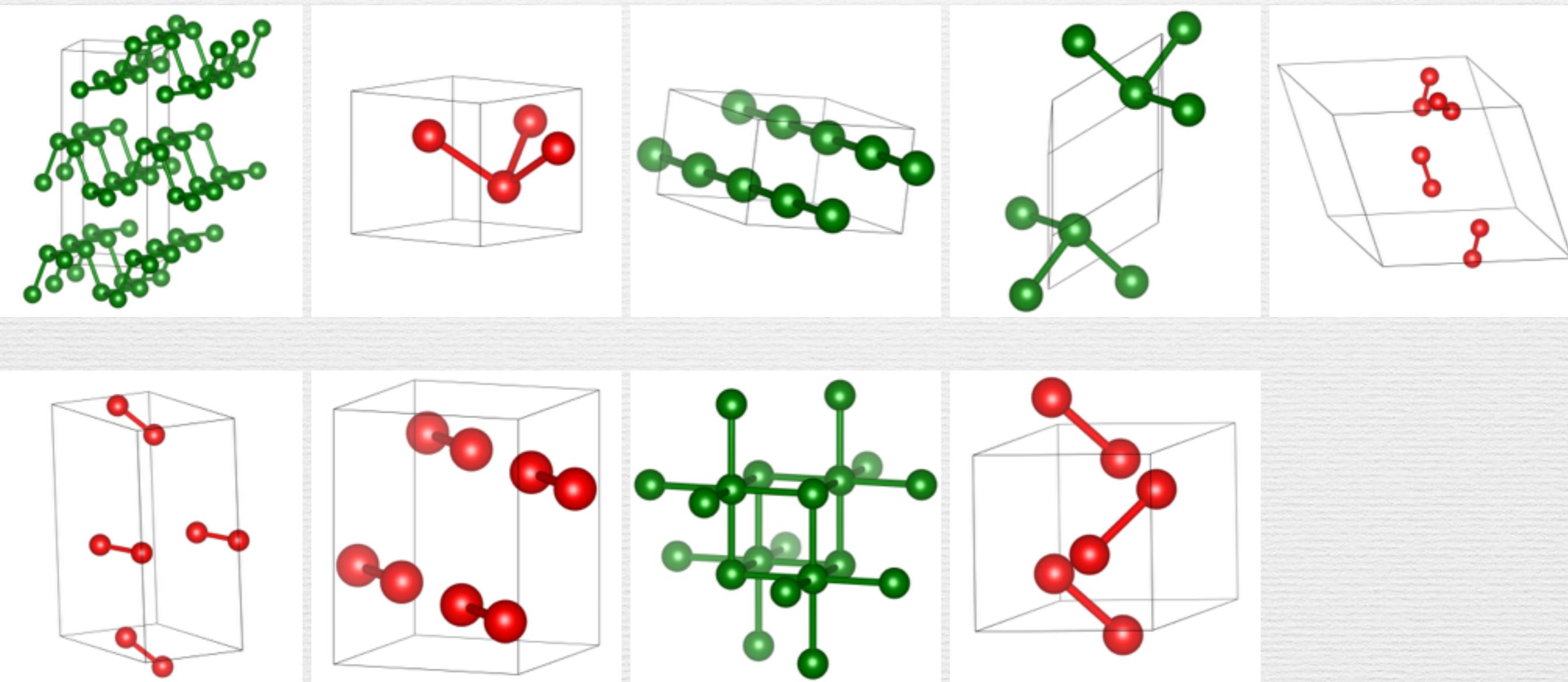


Periodic Systems: Phosphorus Crystals

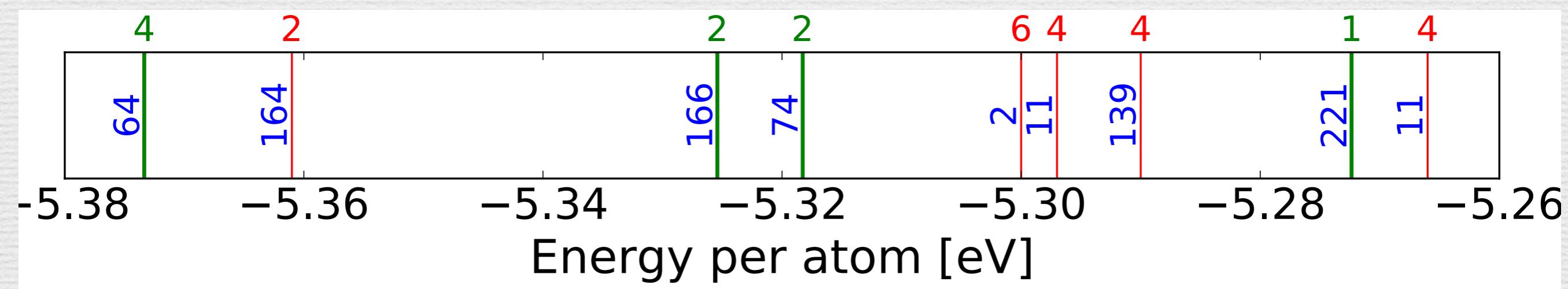
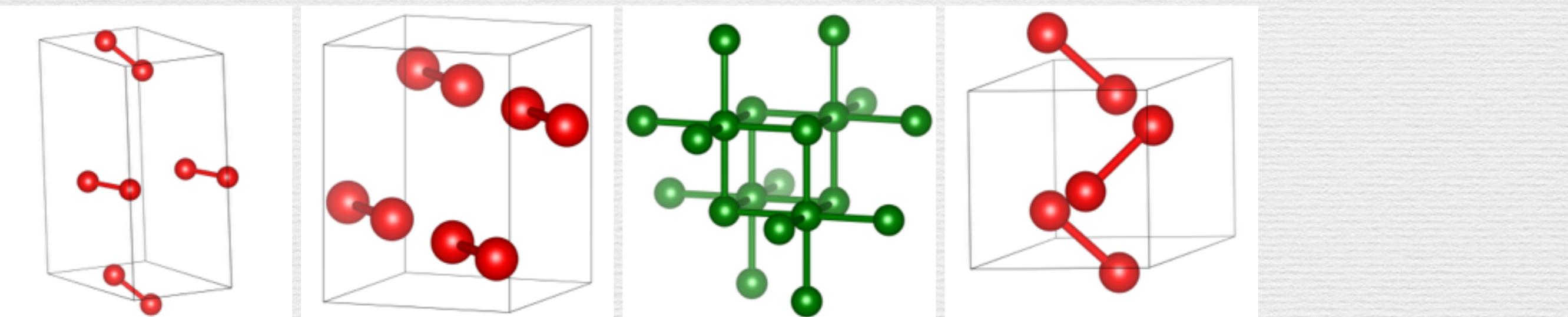
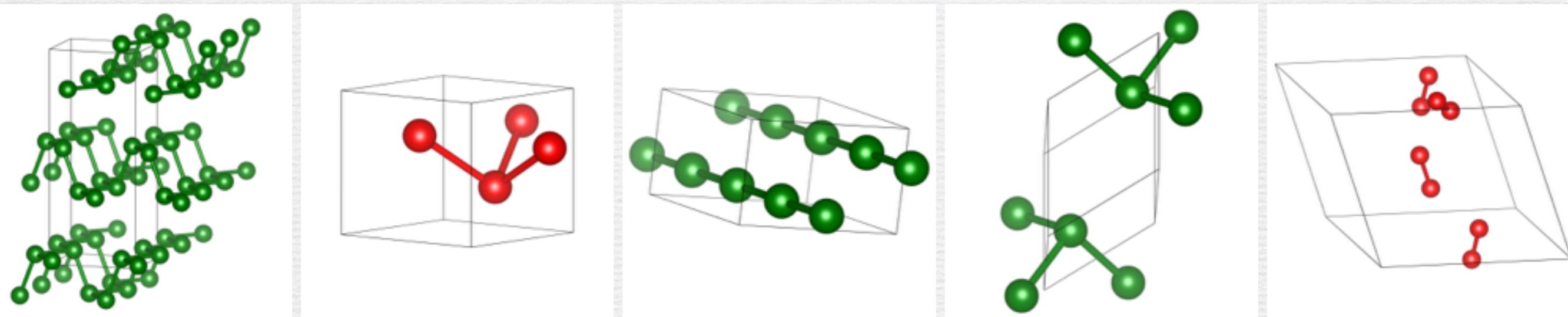
Phosphorus Crystals



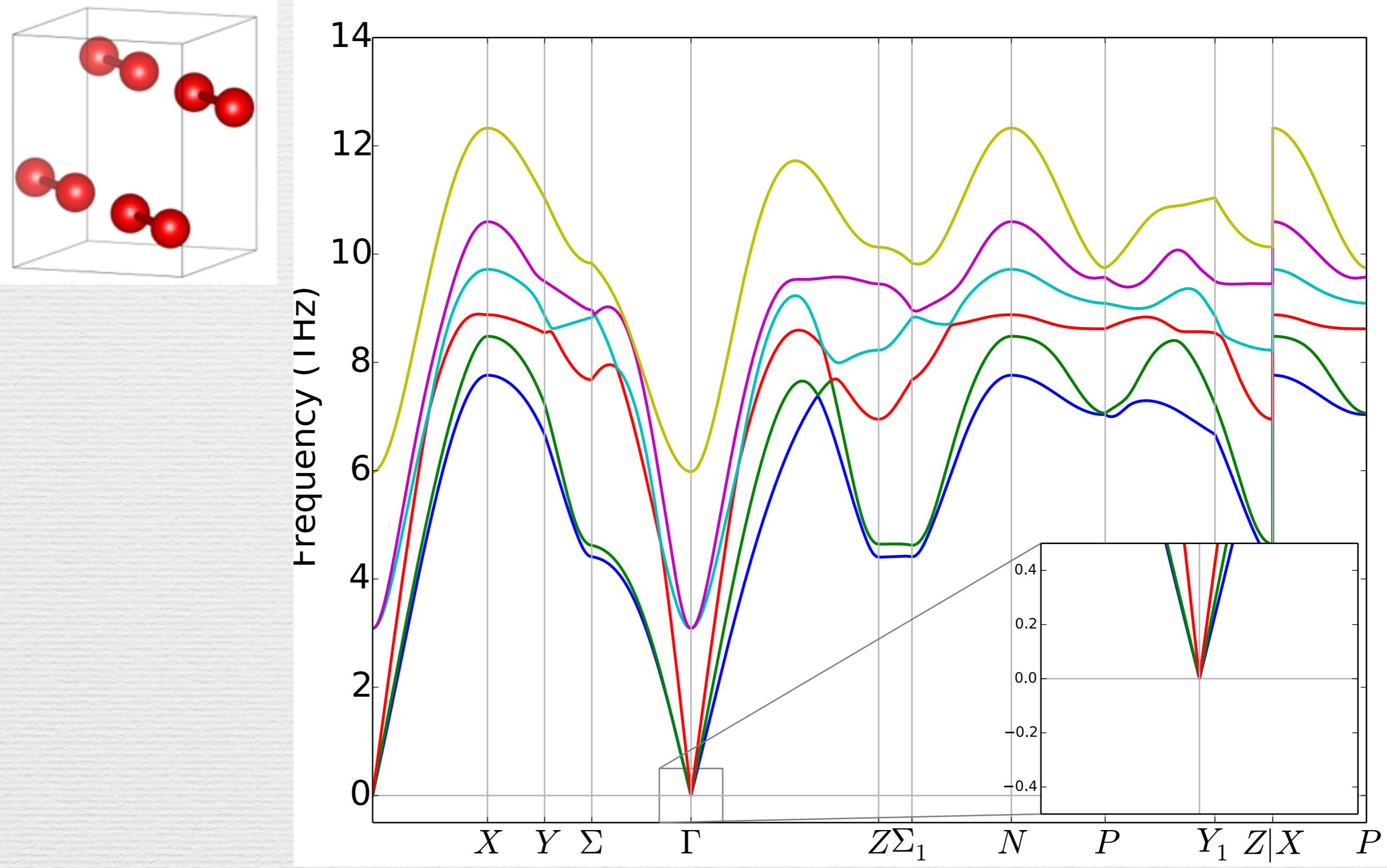
Phosphorus Crystals



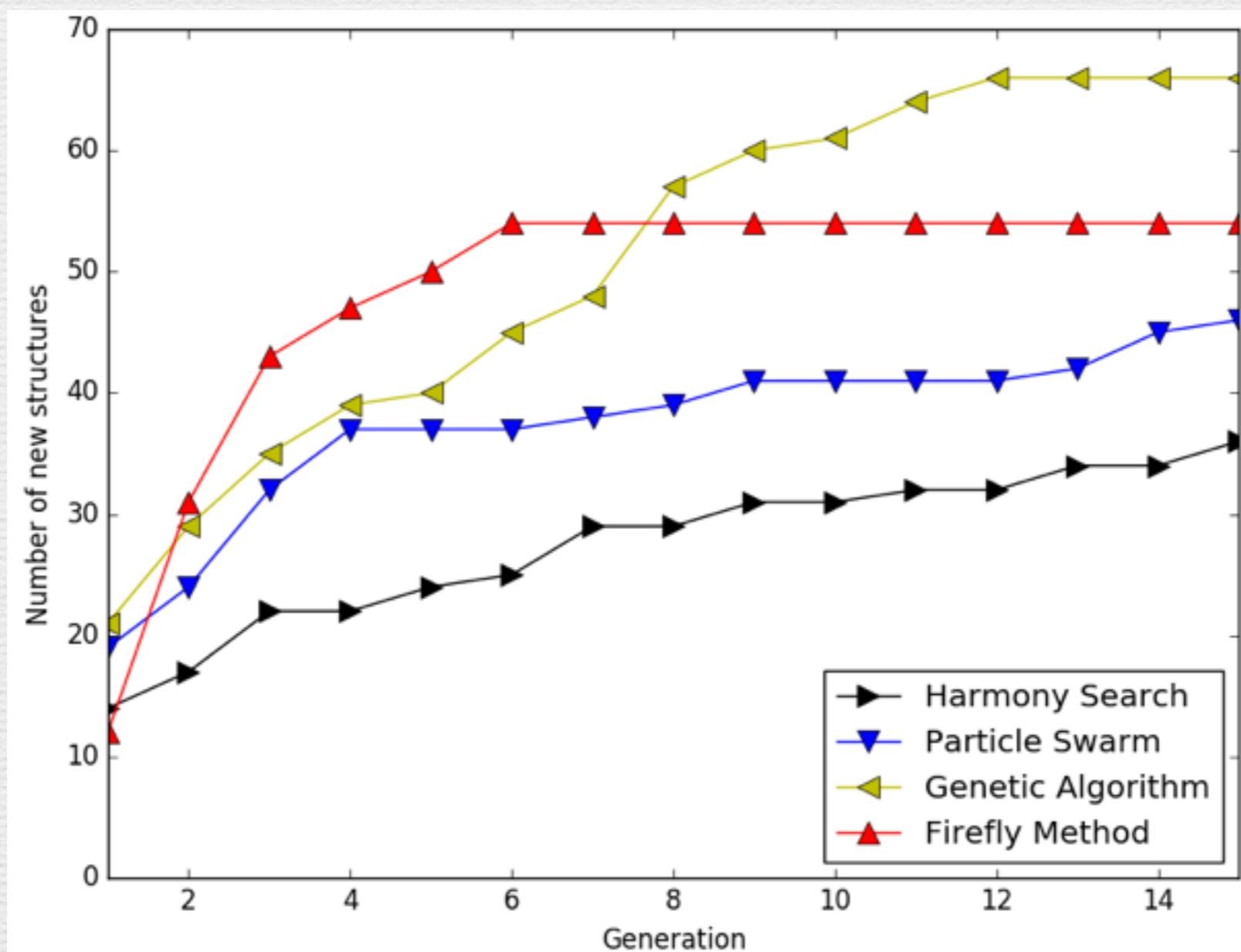
Phosphorus Crystals



Phosphorus Crystals

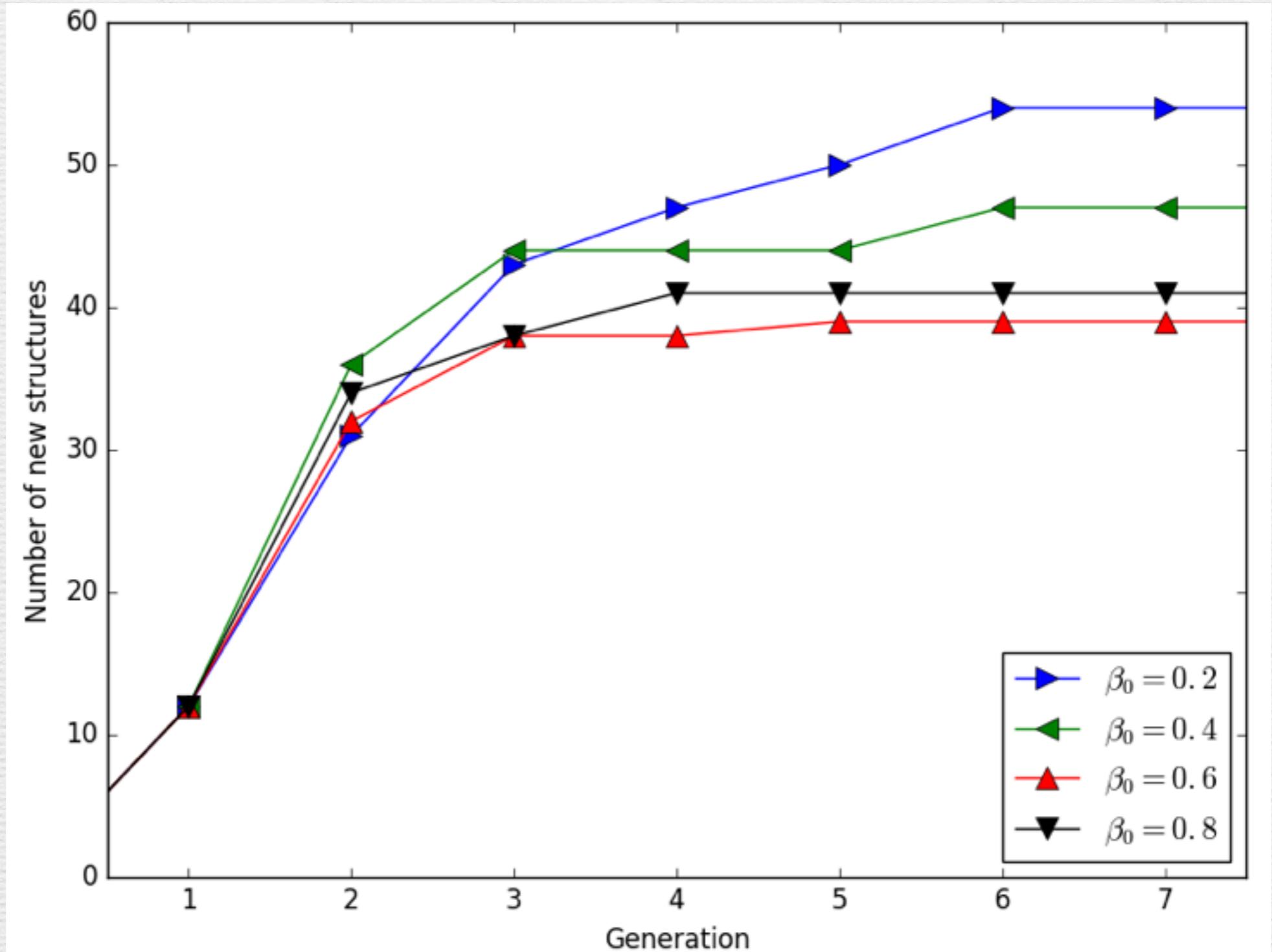


Compared with other metaheuristics

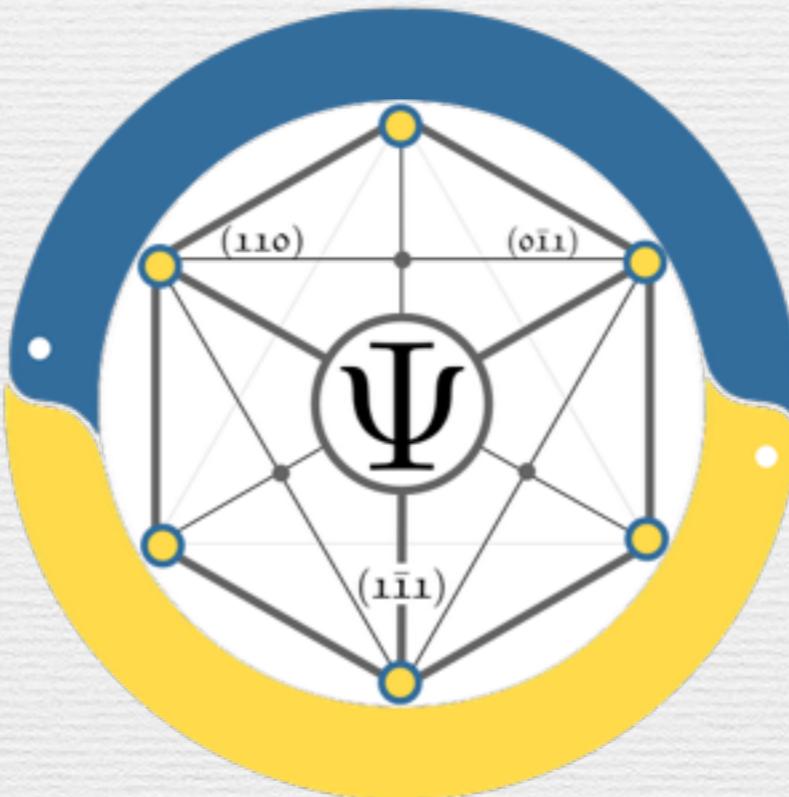


The parameters of Firefly

β_0
 γ
 α_0



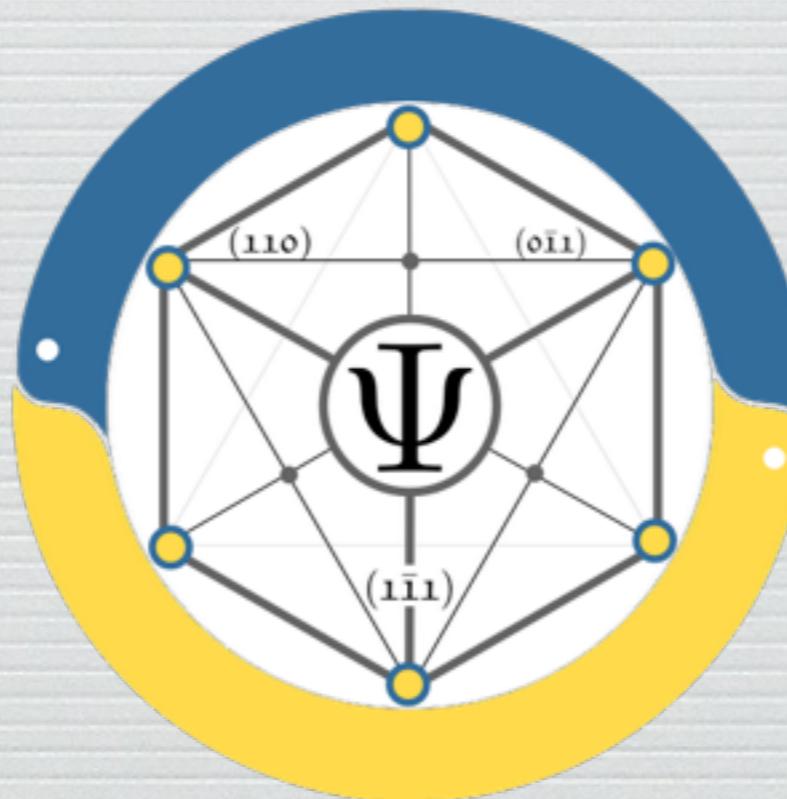
PyChemia



<https://github.com/MaterialsDiscovery/PyChemia>

Conclusions

- Firefly is a metaheuristic population-based method that balance target search and exploration.
- Apply the metaheuristic firefly algorithm to the search of minimal energy structures in Lennard-Jones clusters and Phosphorus crystals.
- Present PyChemia, an open-source python library for ab-initio calculations.



Thank you

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<https://github.com/MaterialsDiscovery/PyChemia>

Phosphorus Crystals

