Structural Prediction and Materials Design

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Outline

Motivation

High-throughput and global minima optimization methods

Materials Design

Application

Conclusions

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Inorganic crystals and technology

Inorganic crystals present in many technological applications

- Electronic devices
- Thermoelectrics
- Superconductors
- Heavy industrial applications
- ...

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1. Some applications still miss a proper material
2. Different materials for different applications

How much of the (chemical) world do we actually know?

Inorganic crystals in the ICSD: 210,229

- Alloys
- Duplicates
- Incomplete entries

- 70,000 well defined compounds

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What if none of these materials fits our needs?

Materials prediction

Search space is enormous!

- Systematic experimental synthesis very expensive and time-consuming

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Explore with computer simulations and synthesize only the best candidates

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High-troughtput methods

Nature often chooses the same solution to similar problems

High-troughtput methods

Nature often chooses the same solution to similar problems

- One takes a known structure, change its chemical composition, and hope that this will also be a stable phase for the new composition
- Chemical composition varied by brute force or by ML algorithms

High-troughtput methods

Pros

- Very efficient
- Able to screen thousands of compounds with limited computing resources

High-troughtput methods

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- Very efficient
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Cons

- Impossibility to discover any material with different crystal structure than of similar compounds already contained in the databases

Global Structural Prediction methods

Given the chemical composition of a solid, obtain its ground-state structure

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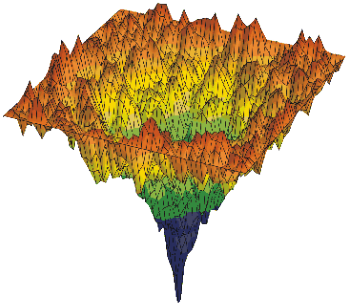

- Potential energy surface (PES): function that gives the energy of a molecule / crystal as a function of its geometry
- Number of possible minima in a solid increases exponentially with the number of atoms

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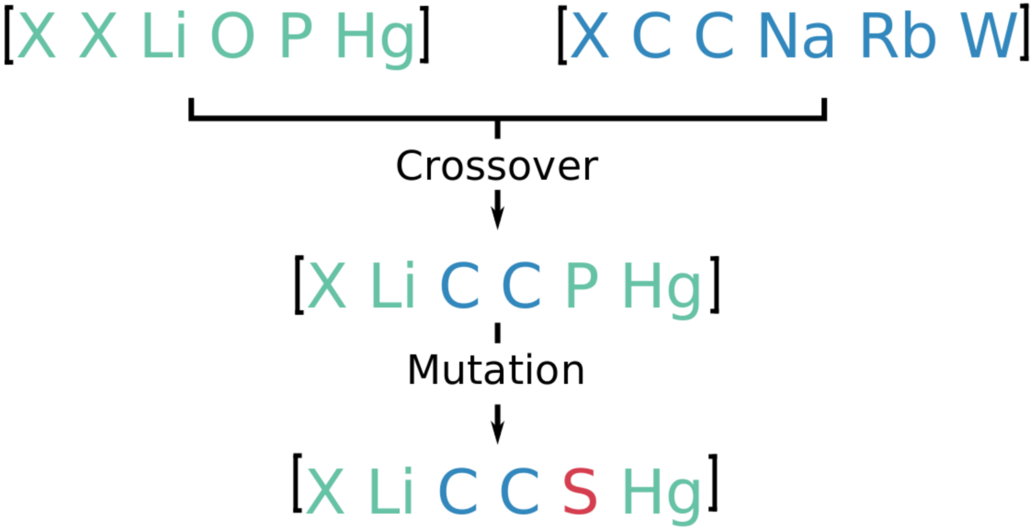
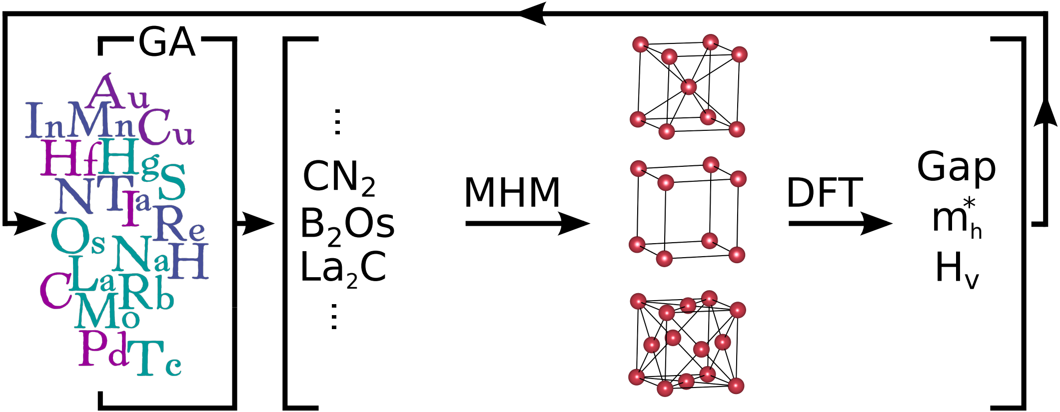
Materials Design

Given a certain property, discover the material that possesses this property

Genetic Algorithms



Materials Design



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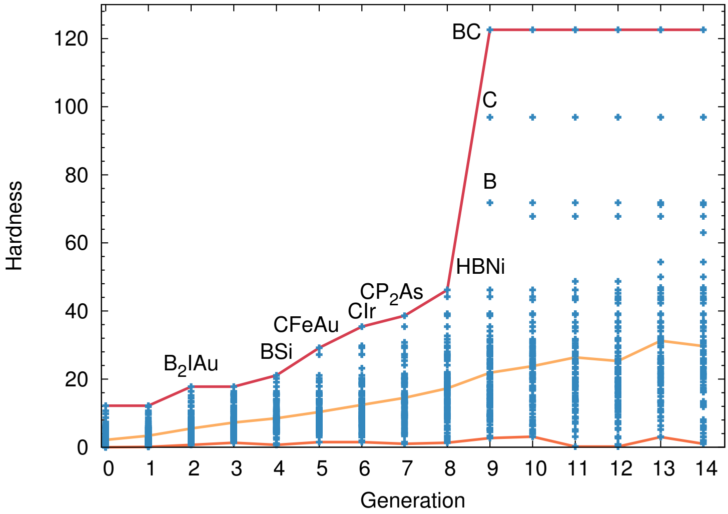
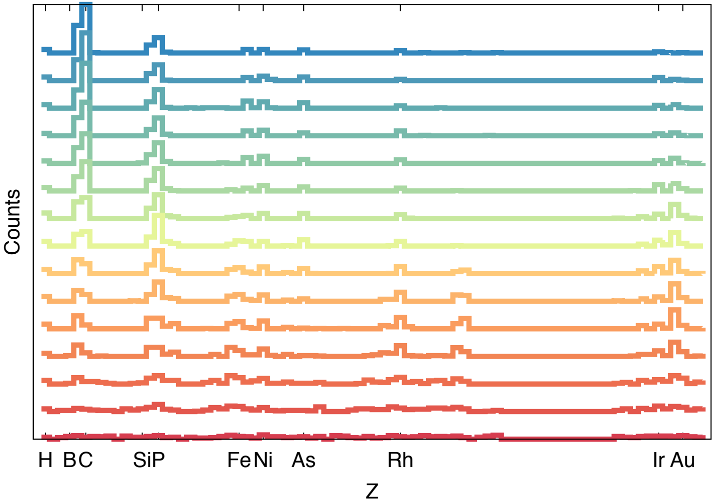
Search for super-hard materials

- Super-hard material: Vickers hardness > 40
- Best known solution is accessible: diamond
- Random initial generation

Search for super-hard materials



Search for super-hard materials



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- Numerical simulations very efficient for materials prediction / screening
- Design materials with tailored properties without any experimentally input
- Efficient with current computer resources
- Completely general: it can be used to design materials optimised for any property(ies)

Thank you

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