Optimizing Lattice Energy in Irregular CM

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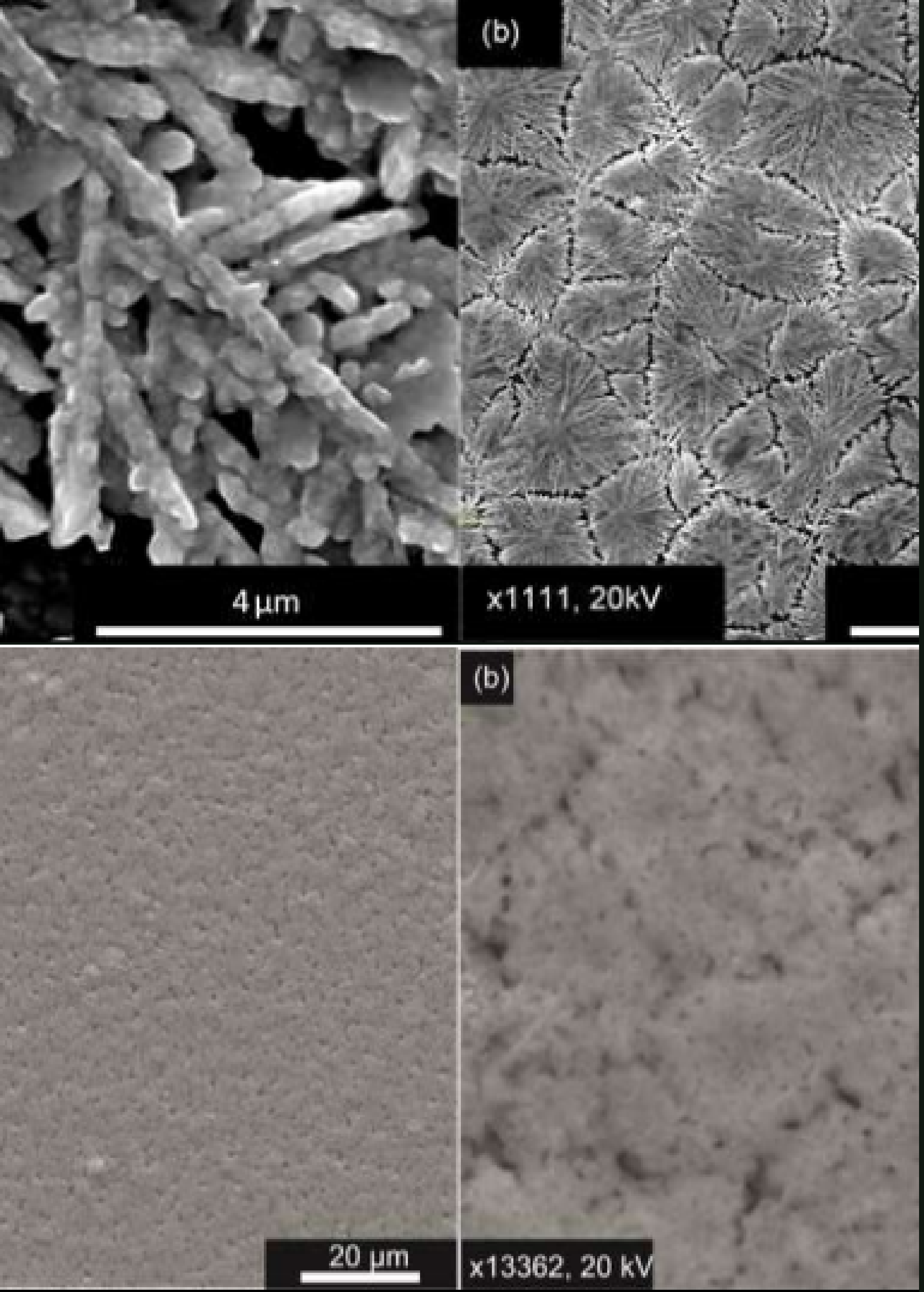

Background

- New lead-free semiconductor Cu_2AgBiI_6 synthesized at University of Liverpool has promising applications in photovoltaics
- Initial research focused on expirimental properties, simulations of internal structure were unoptimized and worth further investigation
- Worth researching: if we're going to put this into a solar panel, we should know its structure!

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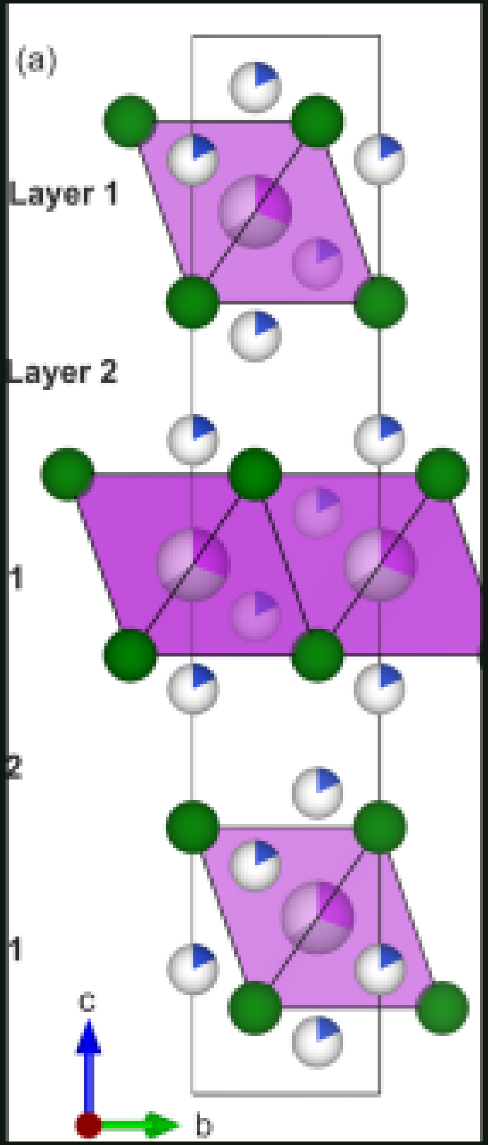

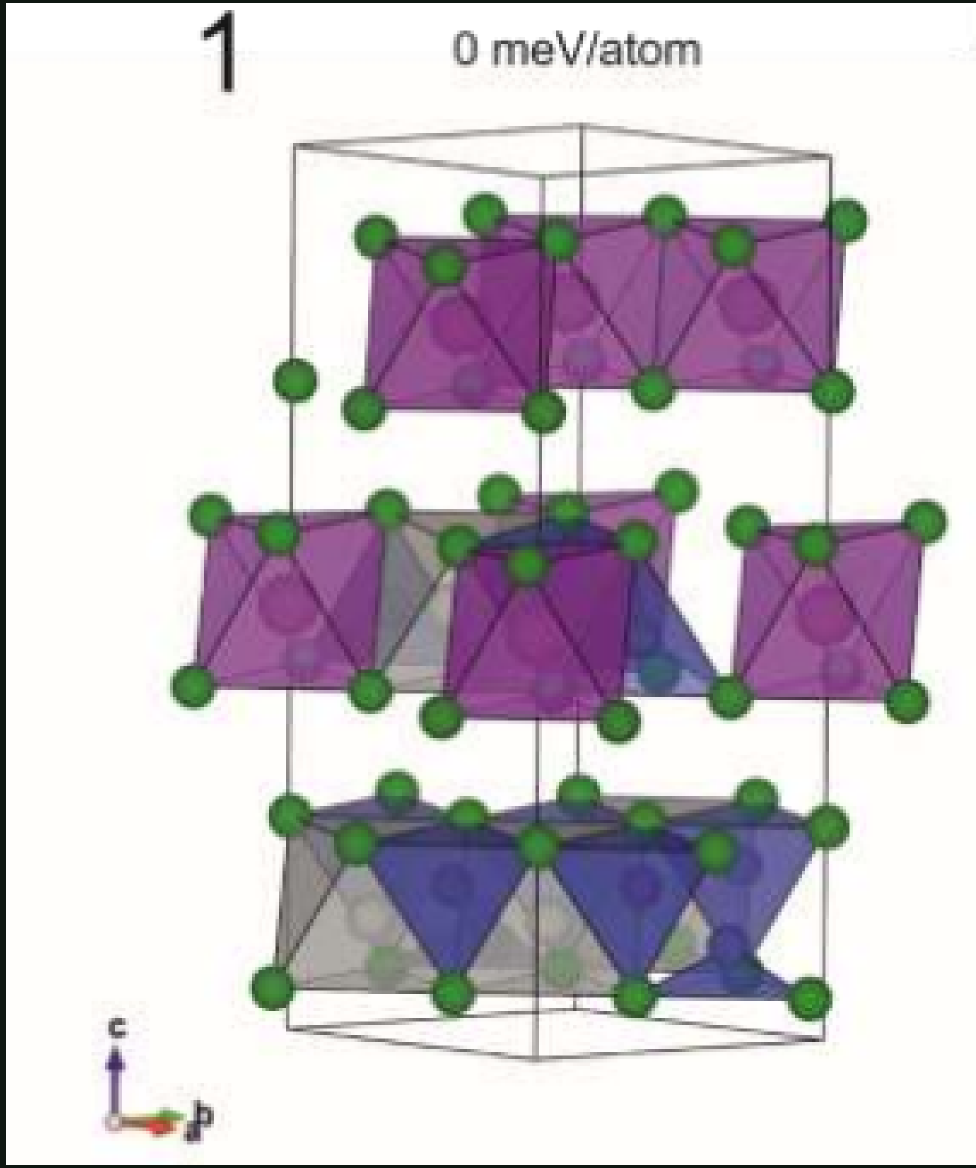

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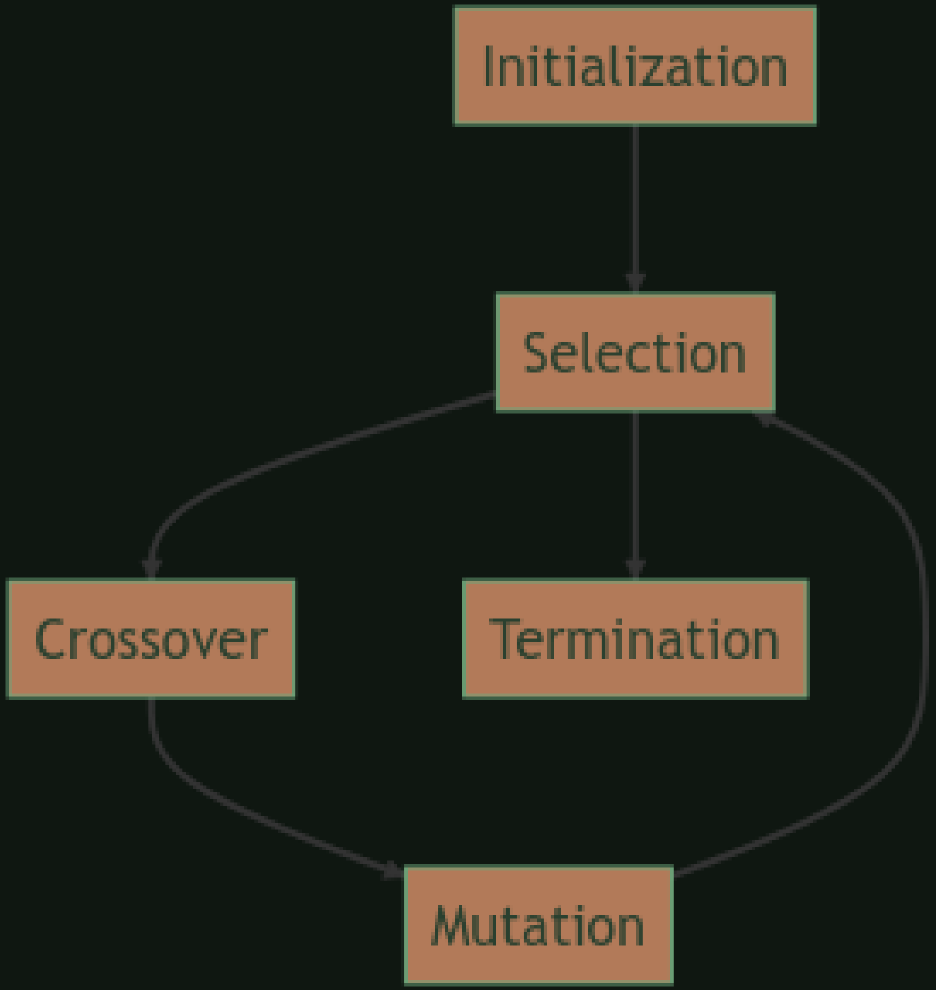
The problem

How can we efficiently find the global minimum of a discrete function with unpredictable behavior and a very large finite domain?

$$\binom{108}{18}\mathrm{Cu} * \left[\binom{27}{9} * \binom{18}{9}\right]\mathrm{Ag/Bi} = 3.173 * 10^{31} \text{ configurations}$$

Big number

- $\mathrm{TB} = 10^{12}$ bytes, would need 4 quintillion 1 TB storage drives to represent each configuration with 1 bit
- In microns, roughly the diameter of the observable universe 🪐🌌



My approach

- Genetic algorithim converges on minimum while only looking at a small sample of the possible configurations
- Easily parallelizable, can run as many simulations as CPU threads available at once
- Use in this field is an active research area, especially with irregular materials

Thank you!

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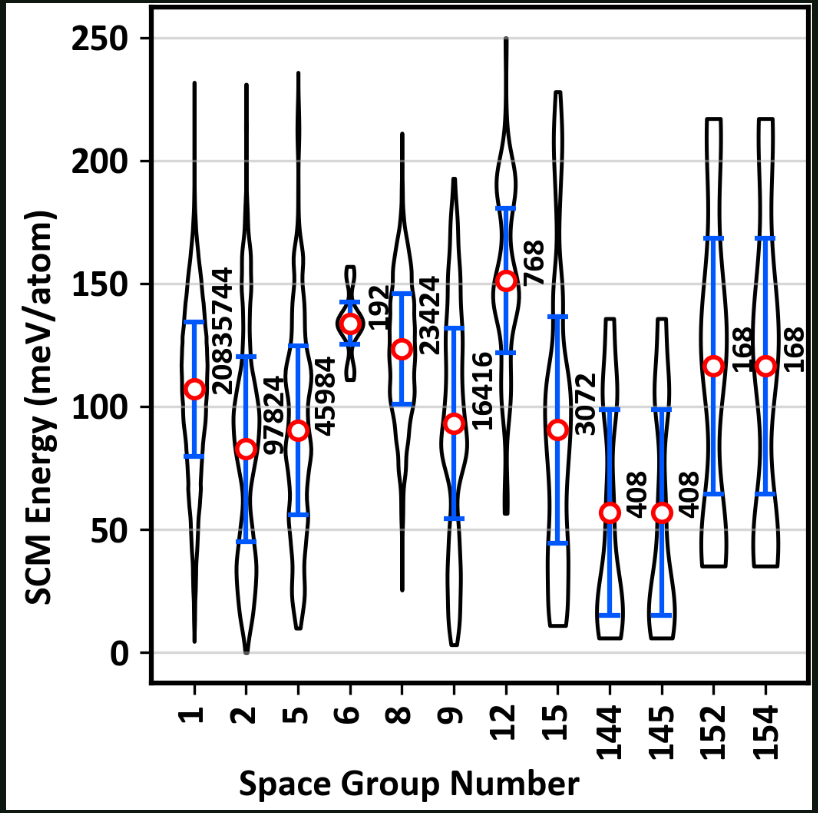
First generation

- Some correlation between crystal symmetry/regularity and lattice energy in similar materials, many exceptions
- Skewing the first generation of configurations towards highly symmetric (high space group) configurations could lead to a faster convergence on a minimum.
- Accomplish this by binning the randomly generated first generation
    - Each bin is equal size but
    - Number of space groups represented in each bin varies



Generating child configurations

- Configs for future generations are generated from the best of the previous generation
- Crossover: site filling is determined by indexing the occupied sites of the parents and selecting at random
- Mutation: A few occupied atomic sites in the child configuration will be swapped with ones chosen at random, most often resulting in an atom switching with a vacancy.