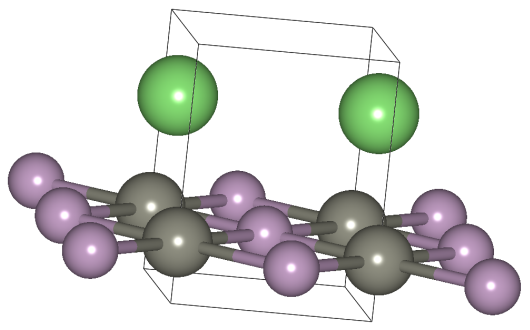
AIRSS

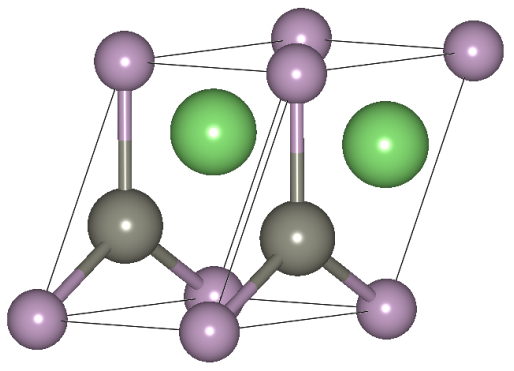
Take a set of atoms

RANDOMISE

With some sensible constraints

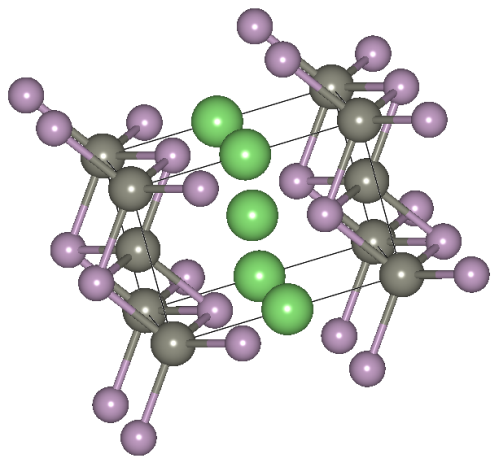


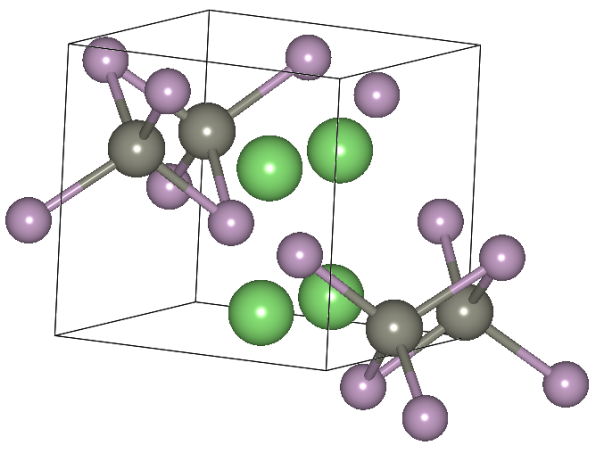
Calculate the energy of the cell



RELAX

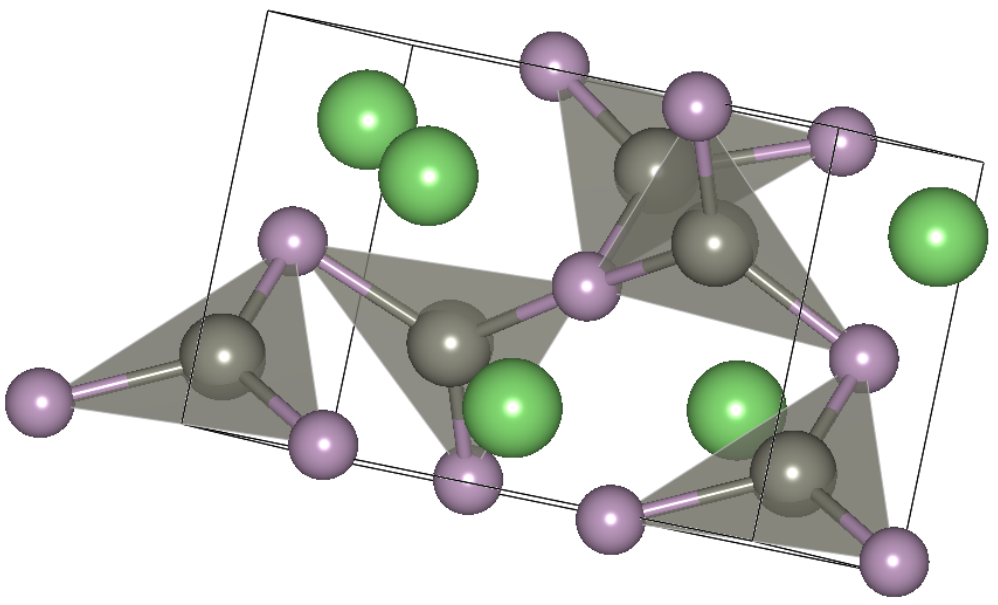
Move the atoms to local minima



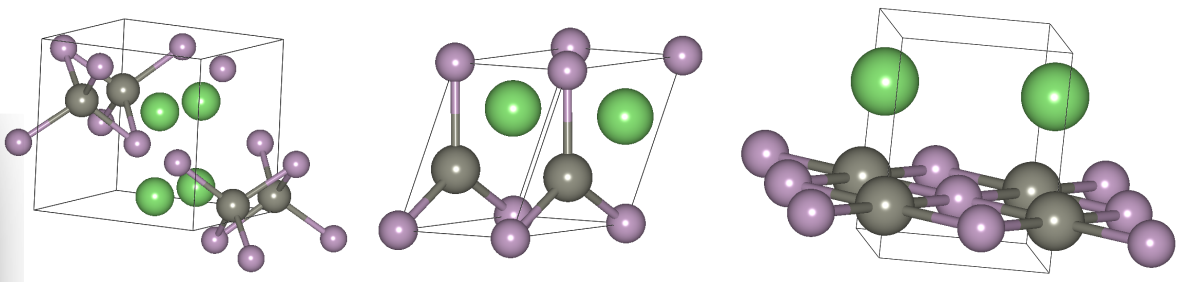


REPEAT

Repeat until the lowest energy structures have been found multiple times



Genetic Algorithm



SEED

Start with random or best guesses as initial popn.

CROSSOVER

Breed two structures by combining periodic cuts of each

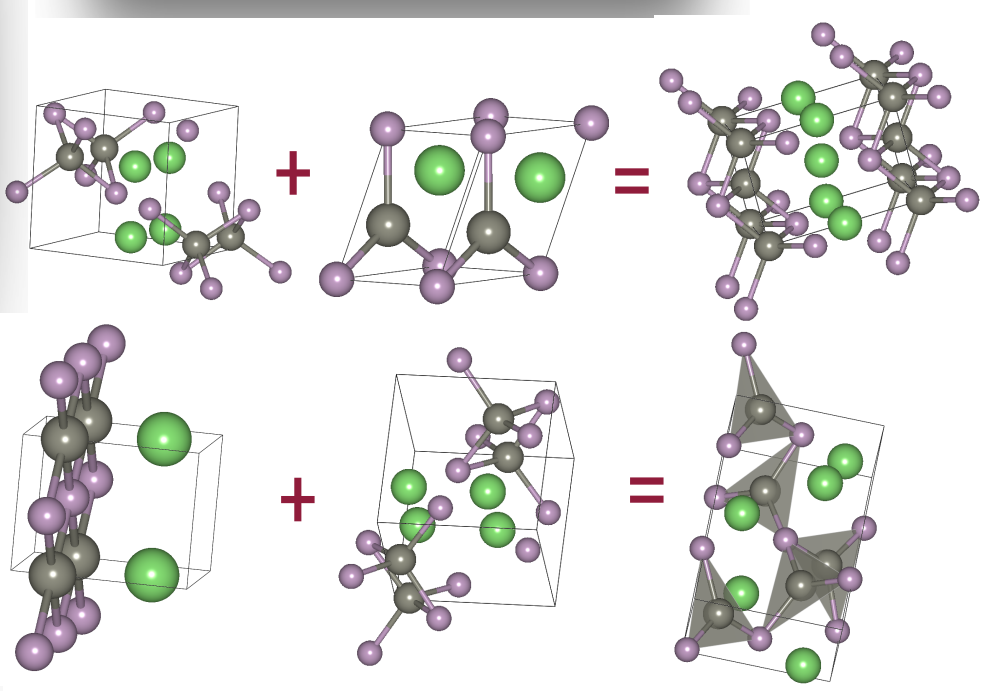
Generate new structures from the current generation

MUTATE

Randomly alter atomic species, positions or lattice

COMPETE

Relax structures with DFT and assess formation energies. Bring only the fittest structures through to the next generation



REPEAT

Repeat for several generations