Genetic Algorithm

SEED

Start with random or best guesses as initial popn.

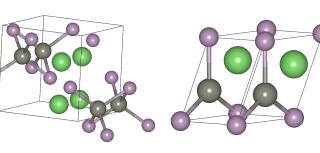
Generate new structures from the current generation

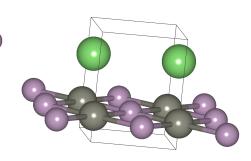
COMPETE

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

REPEAT

Repeat for several generations





CROSSOVER

Breed two structures by combining periodic cuts of each

MUTATE

Randomly alter atomic species, positions or lattice

