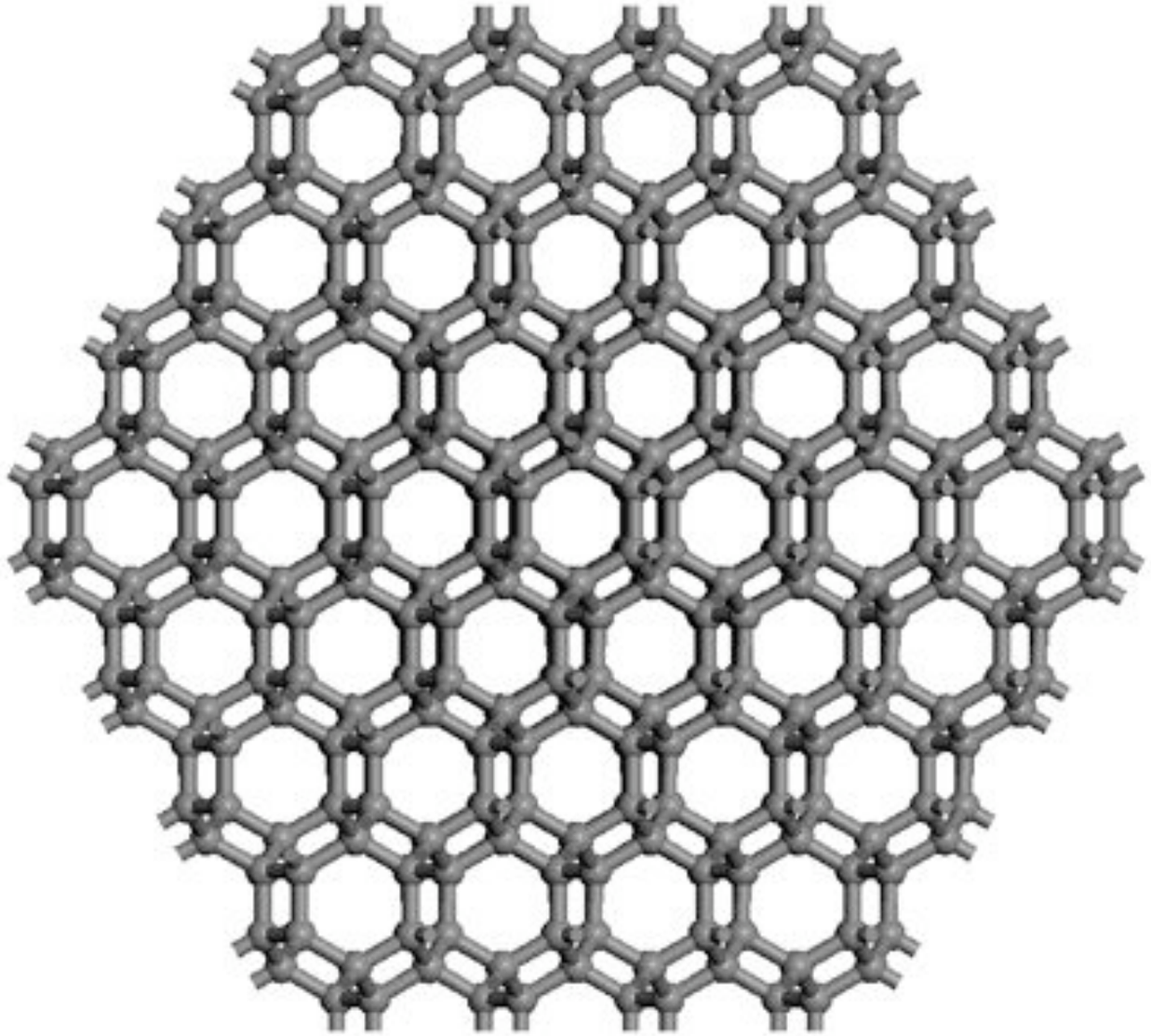
# Random thoughts on structure searching



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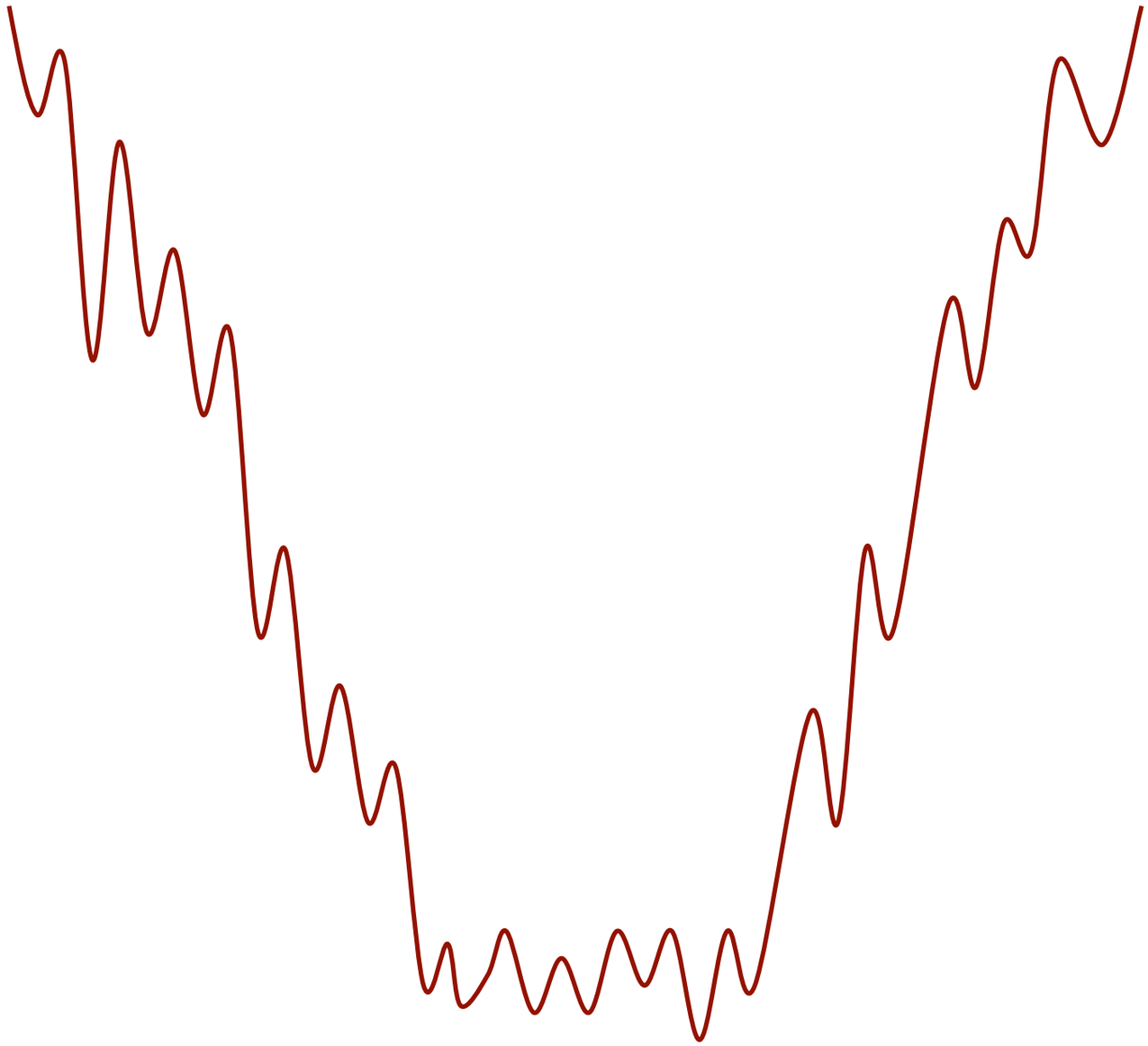
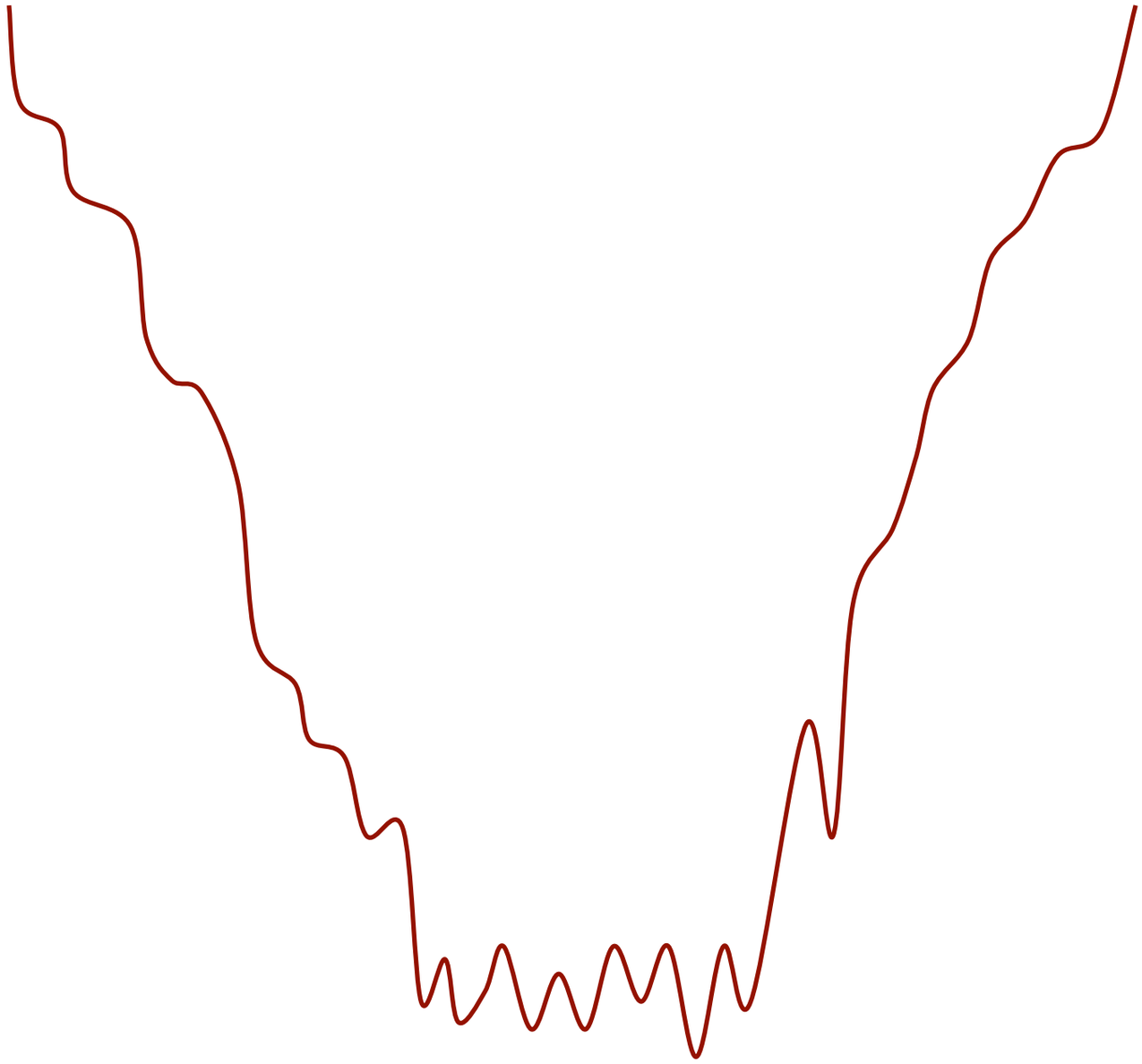
# An obvious question

for condensed matter theory

*What structure will a collection of atoms adopt?*



This a problem of minimisation on a complex energy landscape



Maybe it is not that bad ...

# The "planewaves" of structure search

## The recipe

1. Make a random unit cell

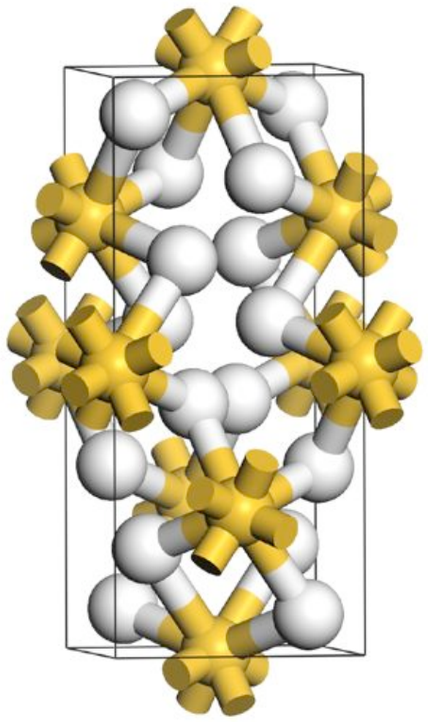
2. Throw a given number of atoms, of given type into the unit cell

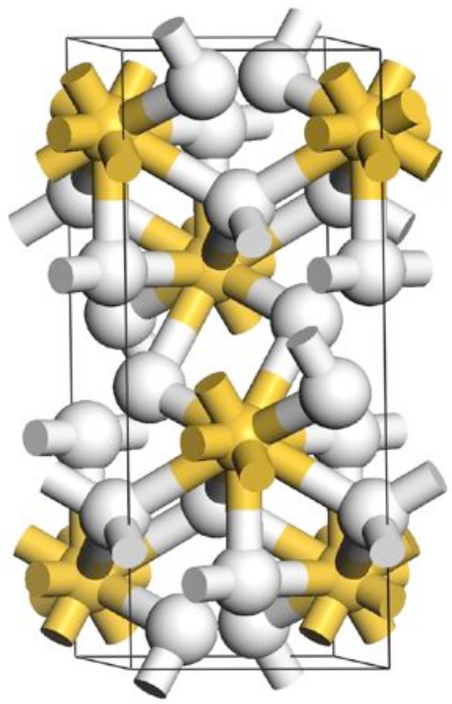
3. Relax carefully under quantum mechanical forces and stress

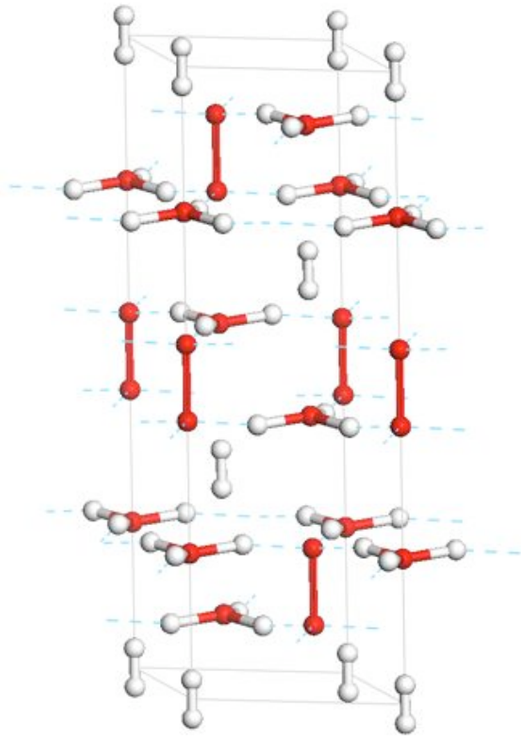
4. Repeat

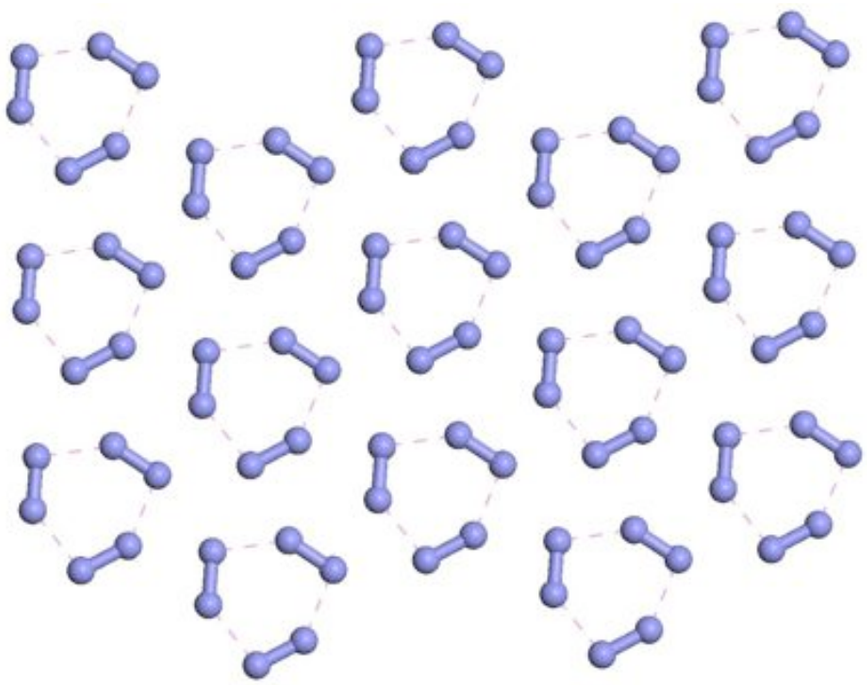
5. Look for lowest energy or most "interesting" structures

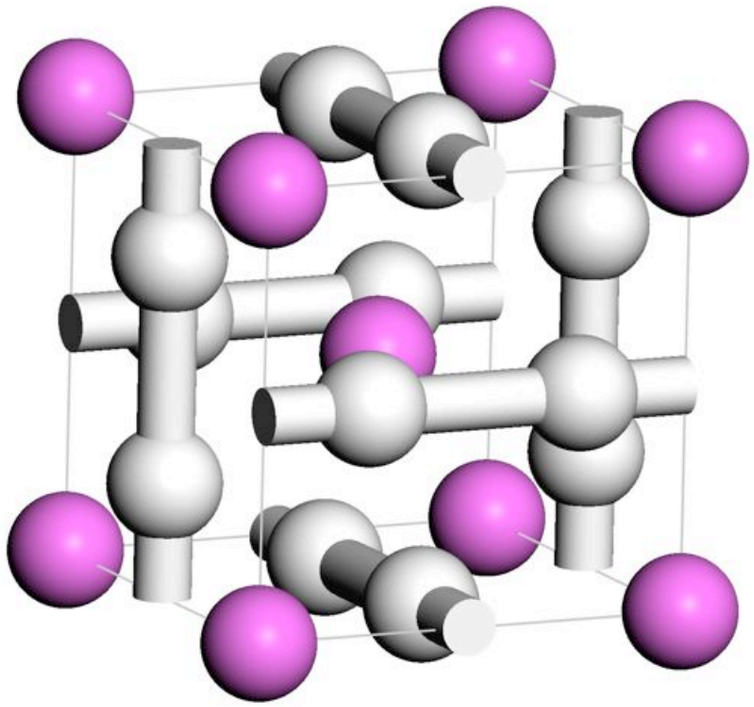
# The proof is in the results





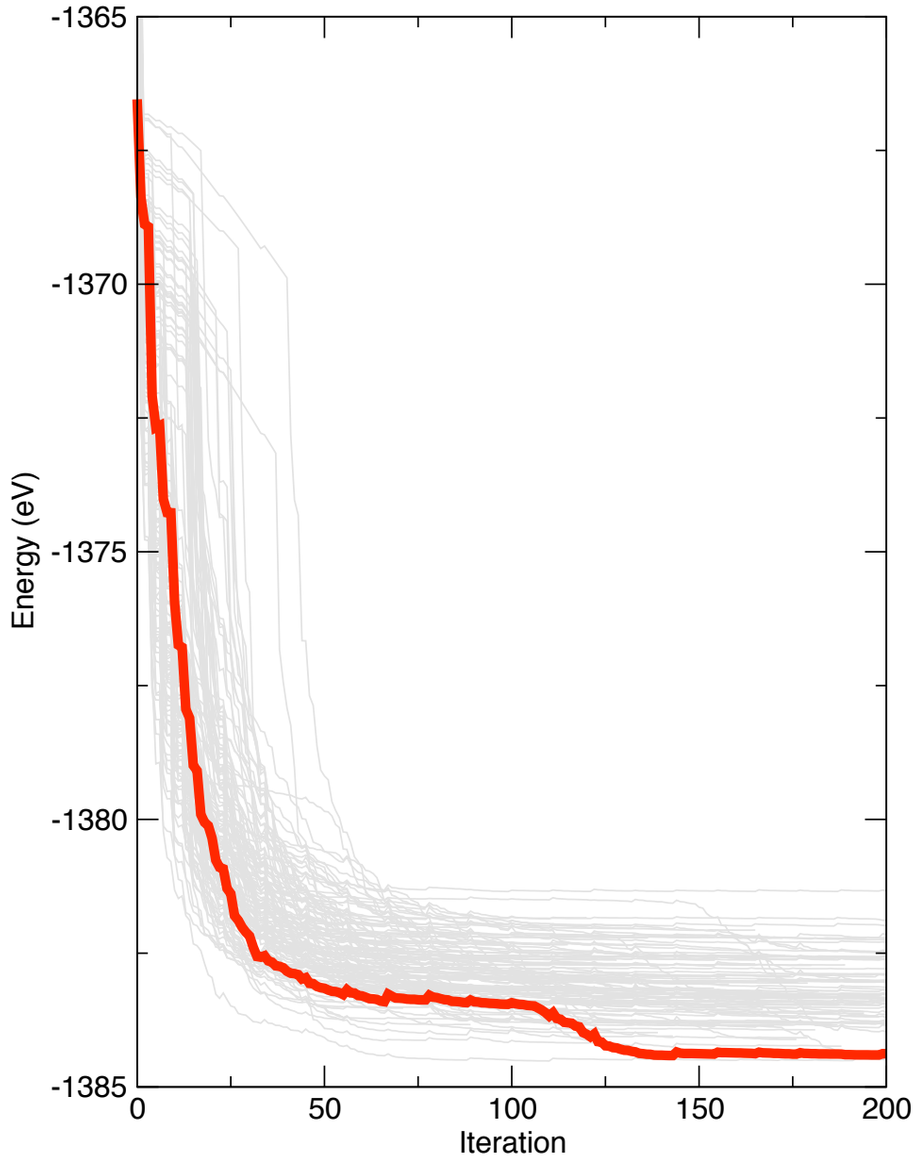






# Is there a free lunch?

"…all algorithms that search for an extremum of a cost function perform exactly the same, when averaged over all possible cost functions. In particular, if algorithm A outperforms algorithm B on some cost functions, then loosely speaking there must exist exactly as many other functions where B outperforms A."
Wolpert and Macready (1995)

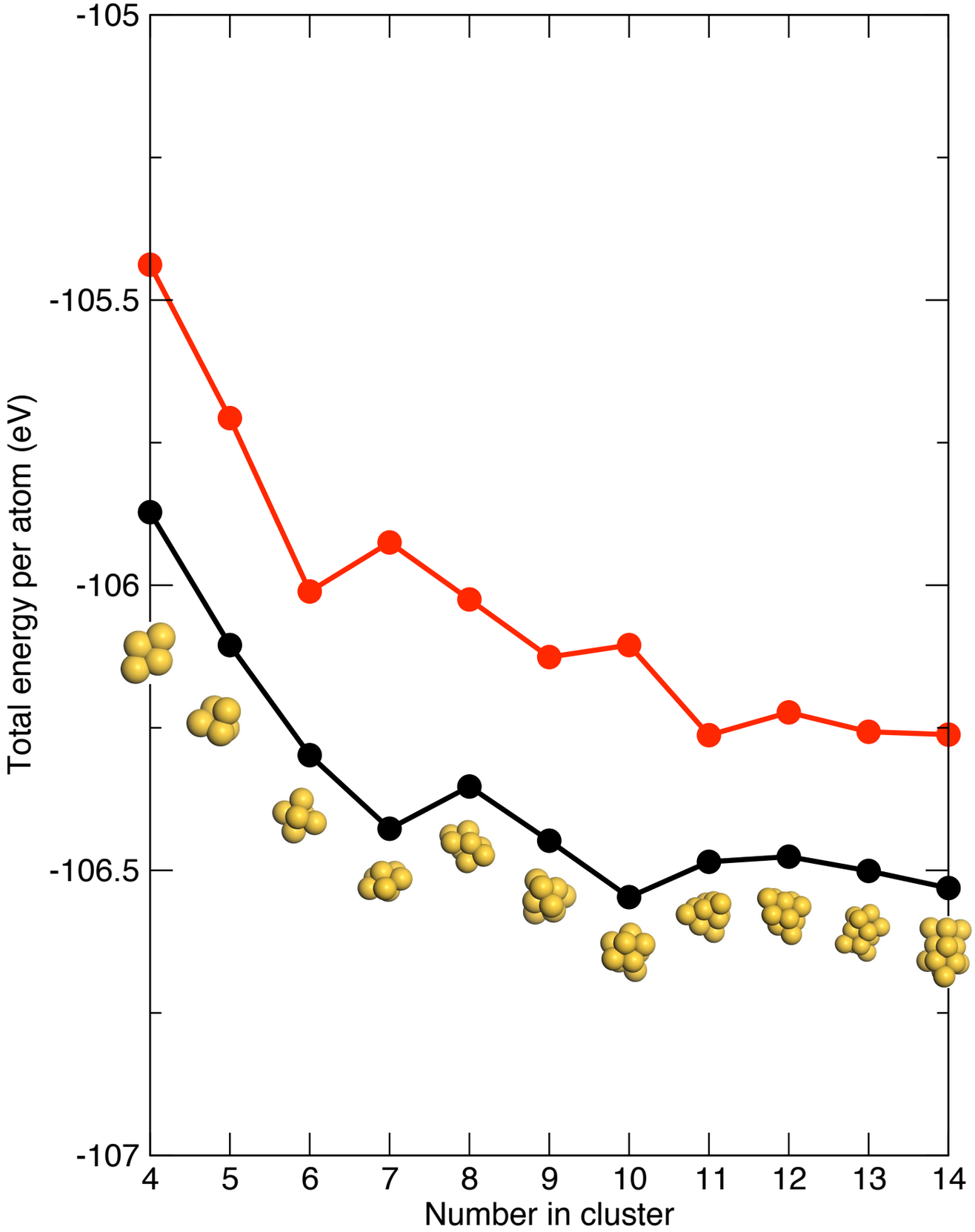


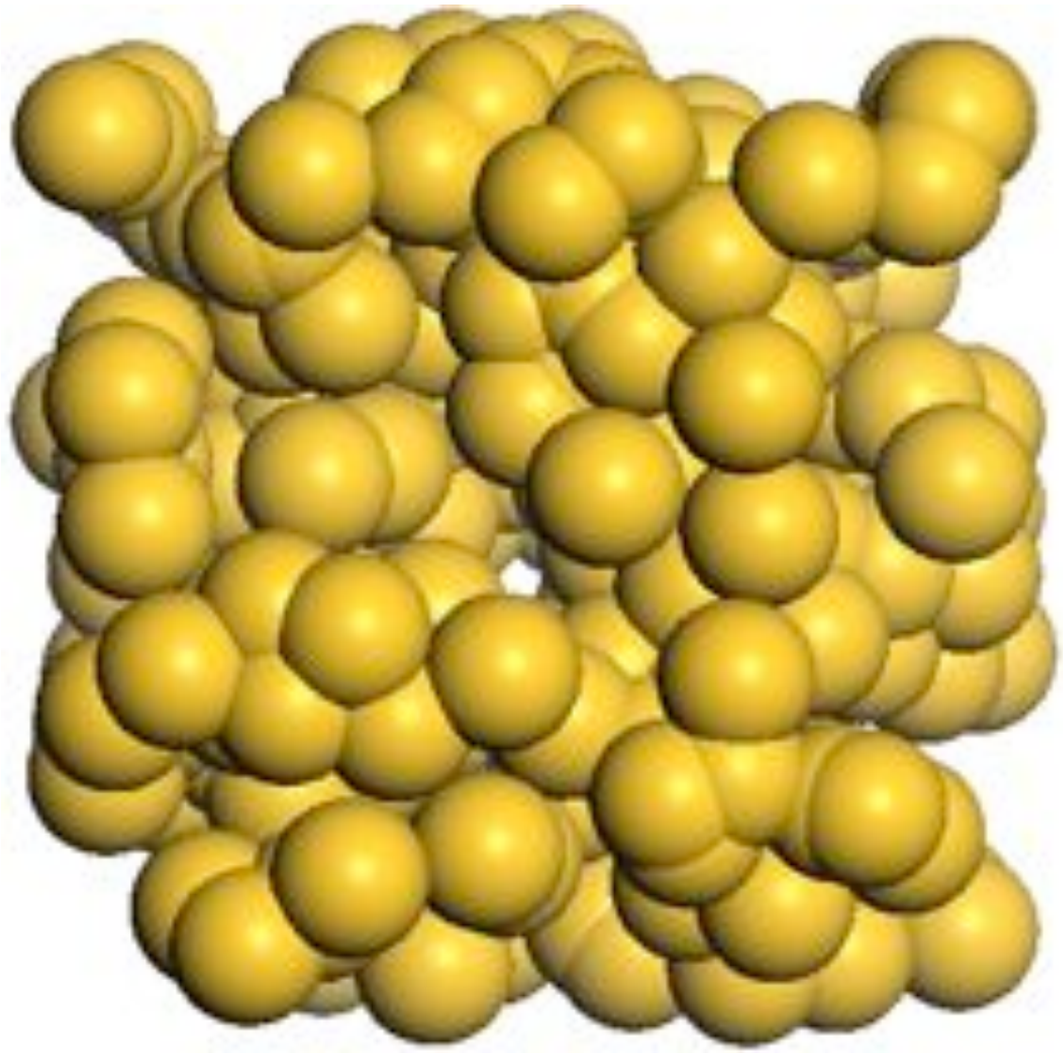

## “Improved” algorithms: genetic algorithms, basin hopping

I think the time is best spent doing science, improving Castep, going to lunch ...

# Silcon clusters

## Maximum and minimum energy structures



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