TCM

Defects in semiconductors using random structure searching

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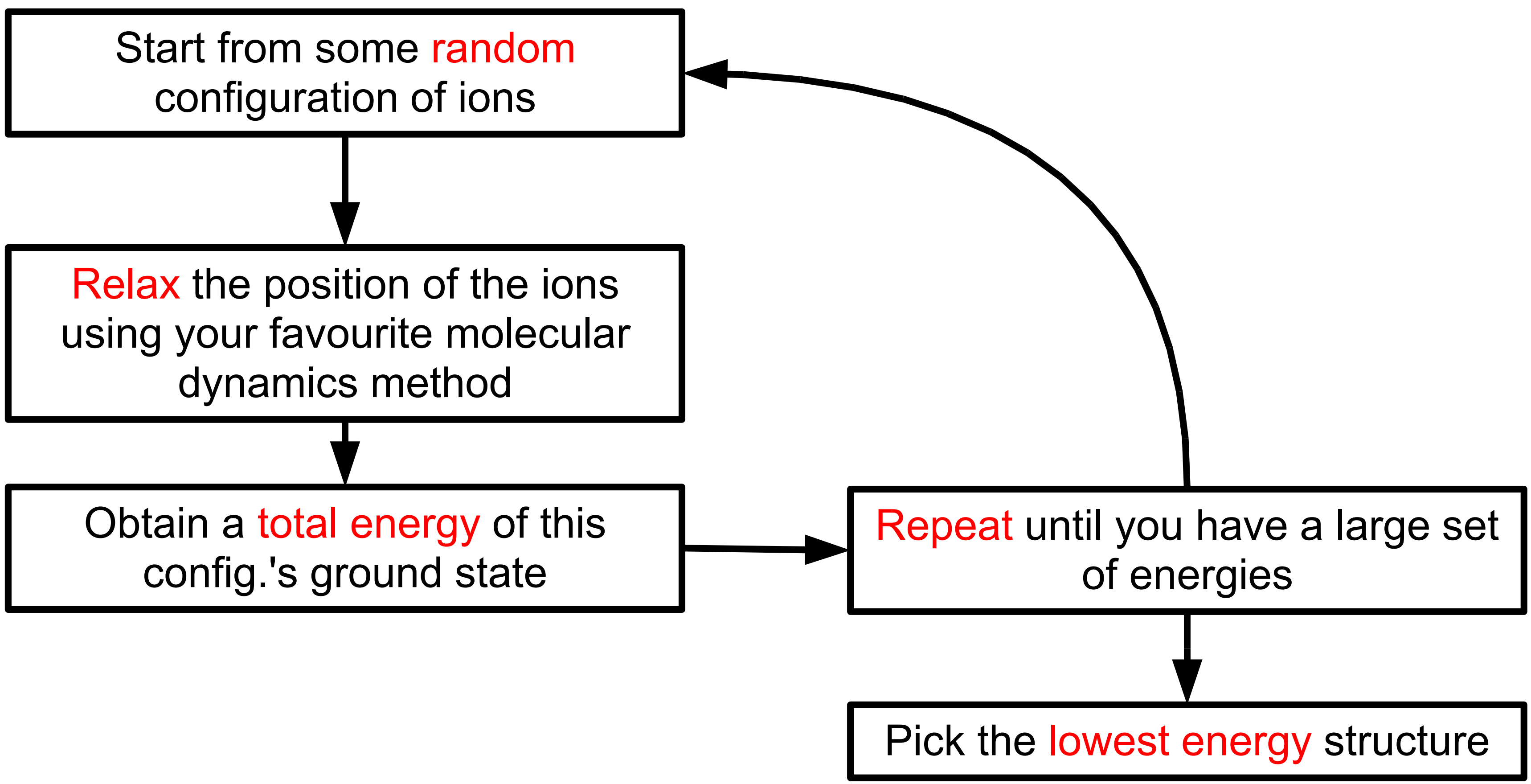
Outline

- What are Random Structure Searches?
- How do we apply them to defect problems?
- Fishing, Polishing and Embedding
- Silicon Self-Interstitials
- Silicon and Hydrogen Intersitials
- Conclusions

What are Random Structure Searches?

- Probably the most simple way to find the lowest energy structure of a solid



Does it work?

- Yes!

- When is H20 not water? CJP + RJN - JCP 2007

- Aluminium Hydride. CJP + RJN – PRB 2007

- Structure of phase III hydrogen. CJP + RJN - Nature Physics 2007

- Graphite interlocation compounds GC + CJP + BDS + RJN – PRB 2007

- High Pressure Silane CJP + RJN – PRL 2006

What about defects in Semiconductors?

- Yes!

  - High Pressure Silane CJP + RJN – PRL 2006

- How do we modify the existing method to get accurate results for semiconductors?

- If we start with every possible config. of the system, we must get the right answer

- Clearly we can't do that!

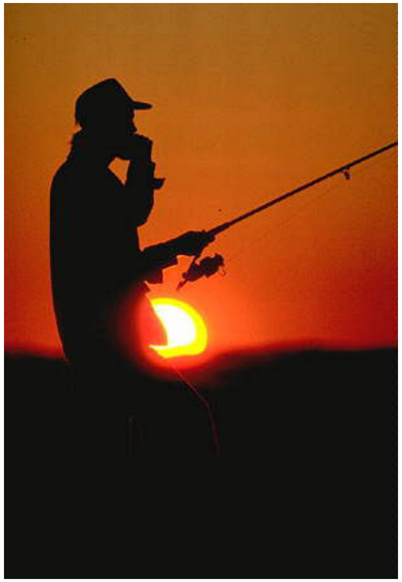
- How do we create starting configs. that constrain the results?

- Make a hole in a perfect lattice ... more later

Method

The Method

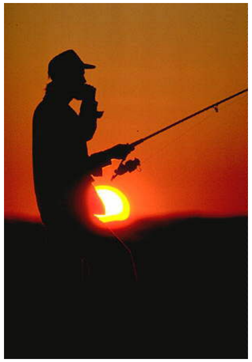
- Fishing



- Polishing

- Embedding

Fishing



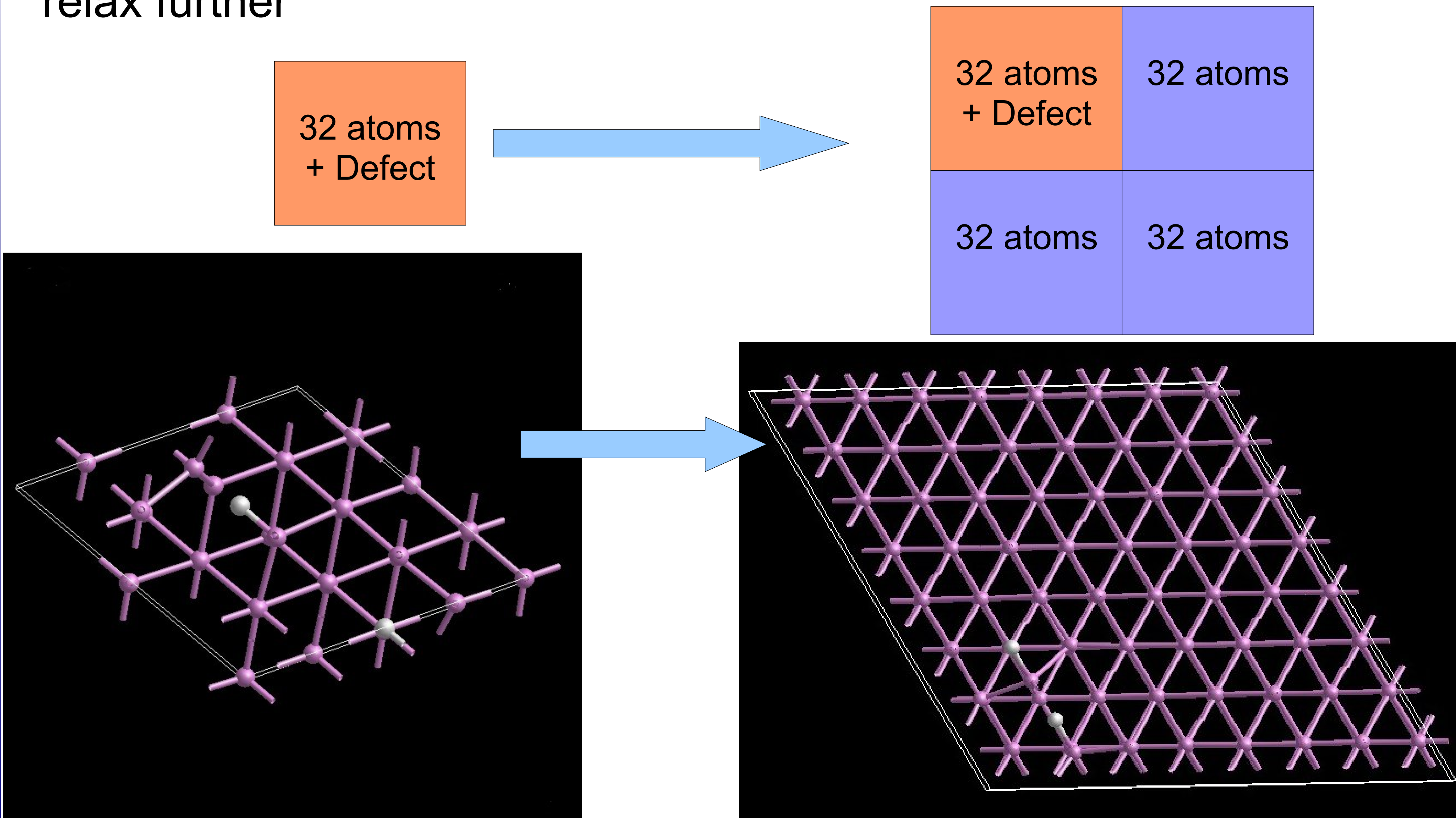
- Catch as many fish as you can.
  - Small cell 32-54 bulk atoms
  - 0.05eV/A force tolerance
  - Darwin
- Don't catch any red herrings.
  - Still has to be accurate =>
    2x2x2 MP grid at Baldereschi Point
    Good pseudopotentials
    DFT
    Fine planewave cutoff
- Know when you've caught whopper.
  - Calculate space group symmetries
  - Good recognition of when two structures are the same

Polishing

- Take:
  - The lowest energy structures
  - The high symmetry structures
  - Anything that looks interesting
- Do more DFT
  - High tolerance relaxation
  - OTF pseudopotentials
- Take similutide.x86
  - See what's well relaxed
  - See what structures are the same
    Even if they have different energies
    Even if they are of low symmetry

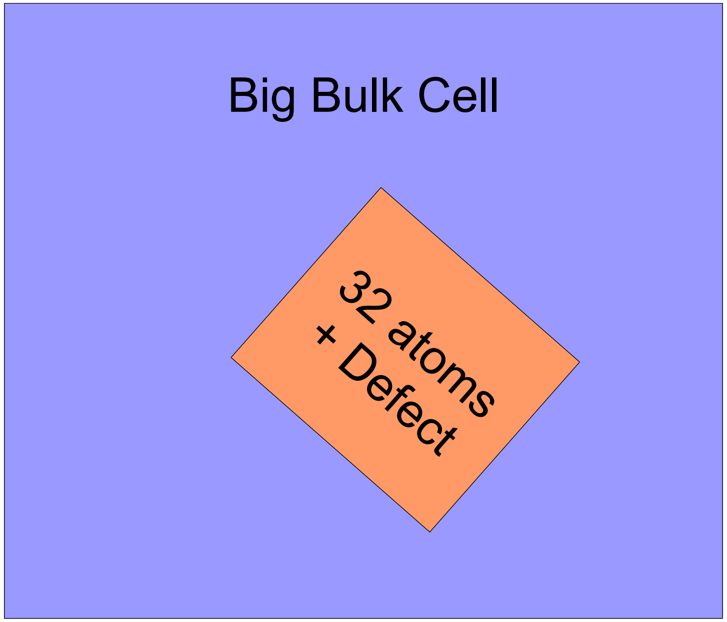
Embedding (1)

- A 32 atom cell is not large enough for an accurate total energy calculation. So we need to put the defect into a larger cell and relax further



Embedding (2)

- This method limits us to 8 times the volume of the defect cell.
- Would like to do:



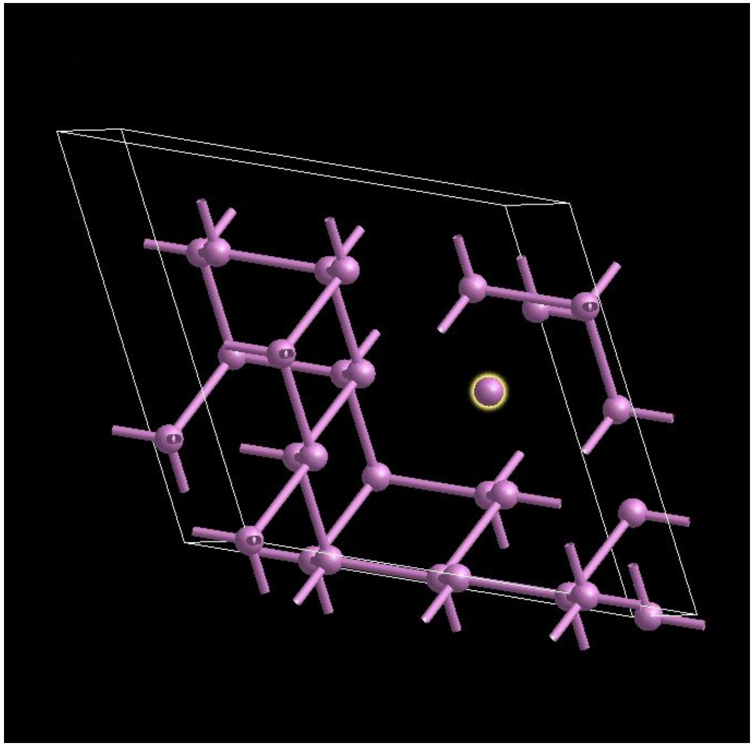
- This is not as easy as it looks. Although I have got a method that works...just a code that doesn't yet!

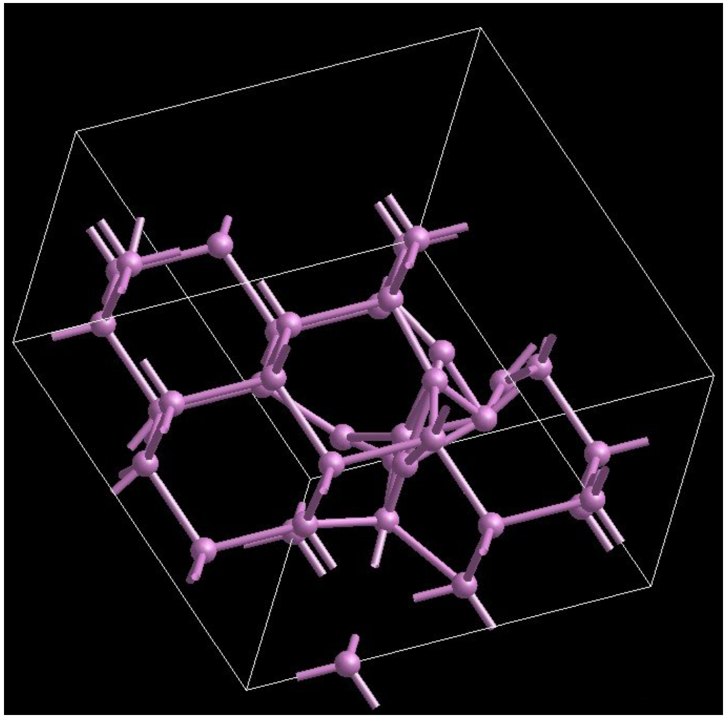
- GEM (General Embedder and Mover) coming soon...

Silicon with Silicon Interstitials

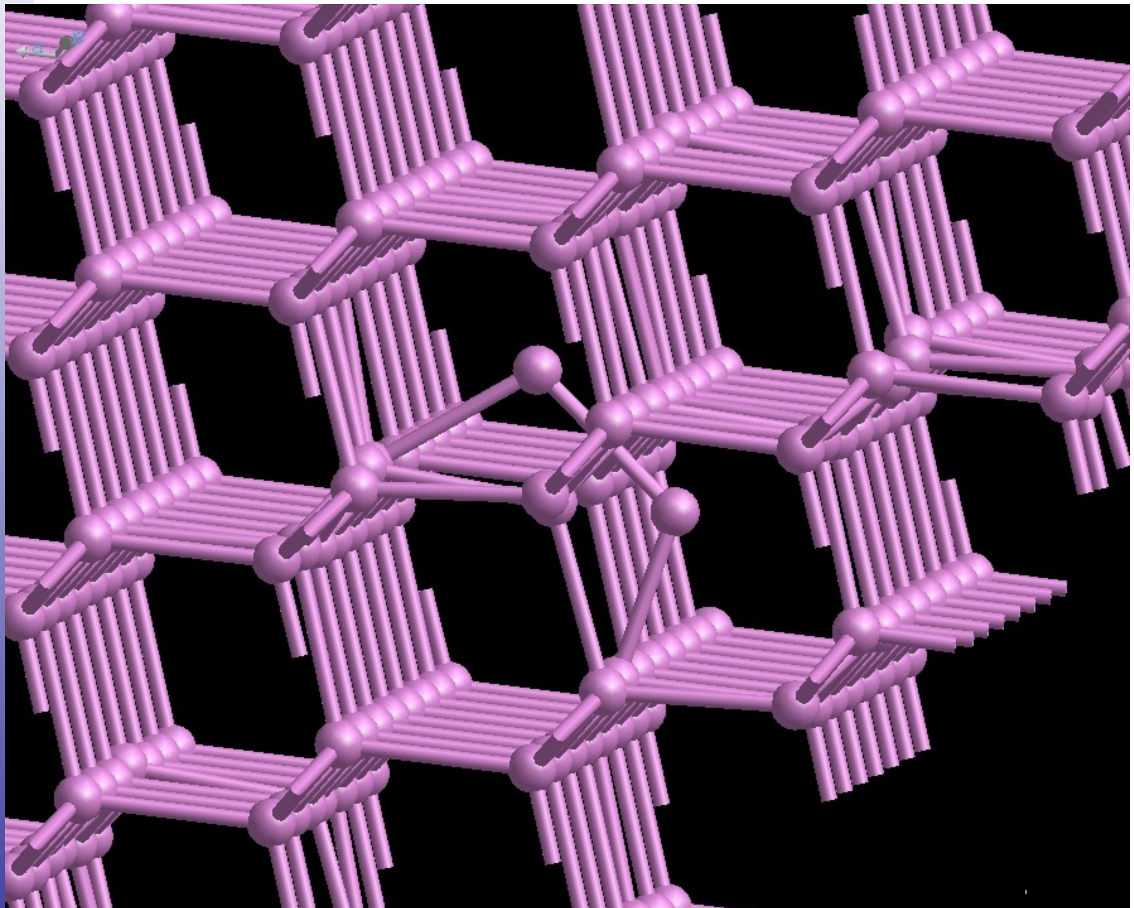
Constraints

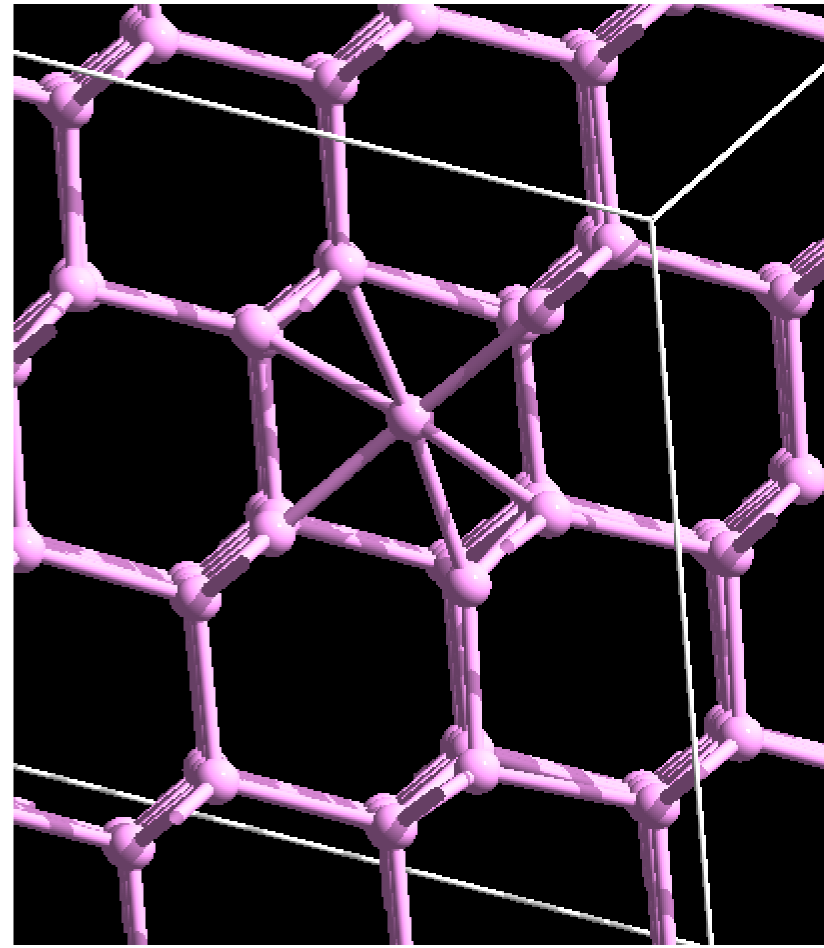
- Want to constrain the search.
- Do this by keeping the bulk intact and creating a hole of randomness.
- For example: Silicon self-interstital
    - Bulk 54 atoms. Plus 1, 2, 3, or 4 extra Silicon atoms.
    - Remove 5 atoms from the bulk
    - Within this hole, randomly place 6 ,7, 8 or 9 atoms.





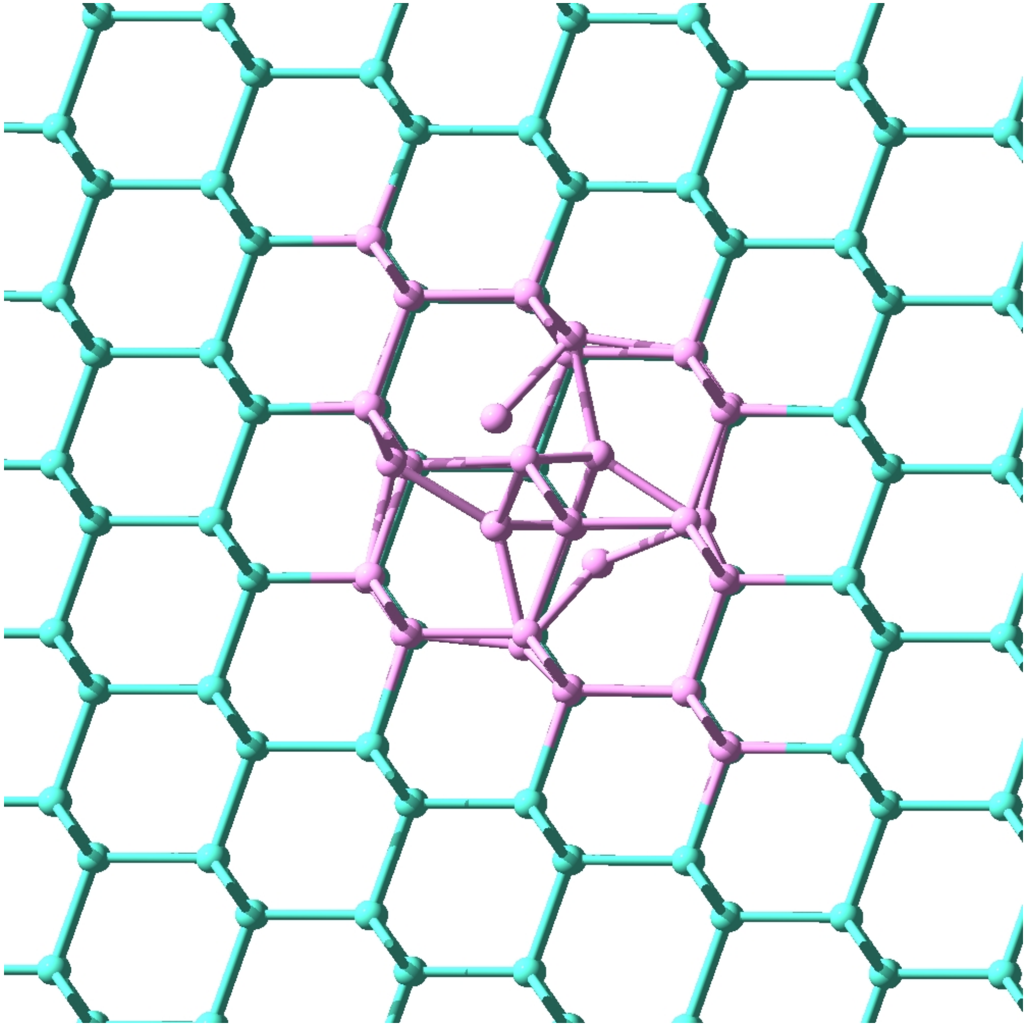
Silicon with 1 extra Silicon





- Find both ground state structures quite easily.

Silicon with 4 extra Silicon



- Lowest energy
- Problem, the search cell was too small. Don't get a true ground state

Silicon with Silicon and Hydrogen Interstitials

Silicon with 1 extra Silicon and 1,2,3 or 4 Hydrogen

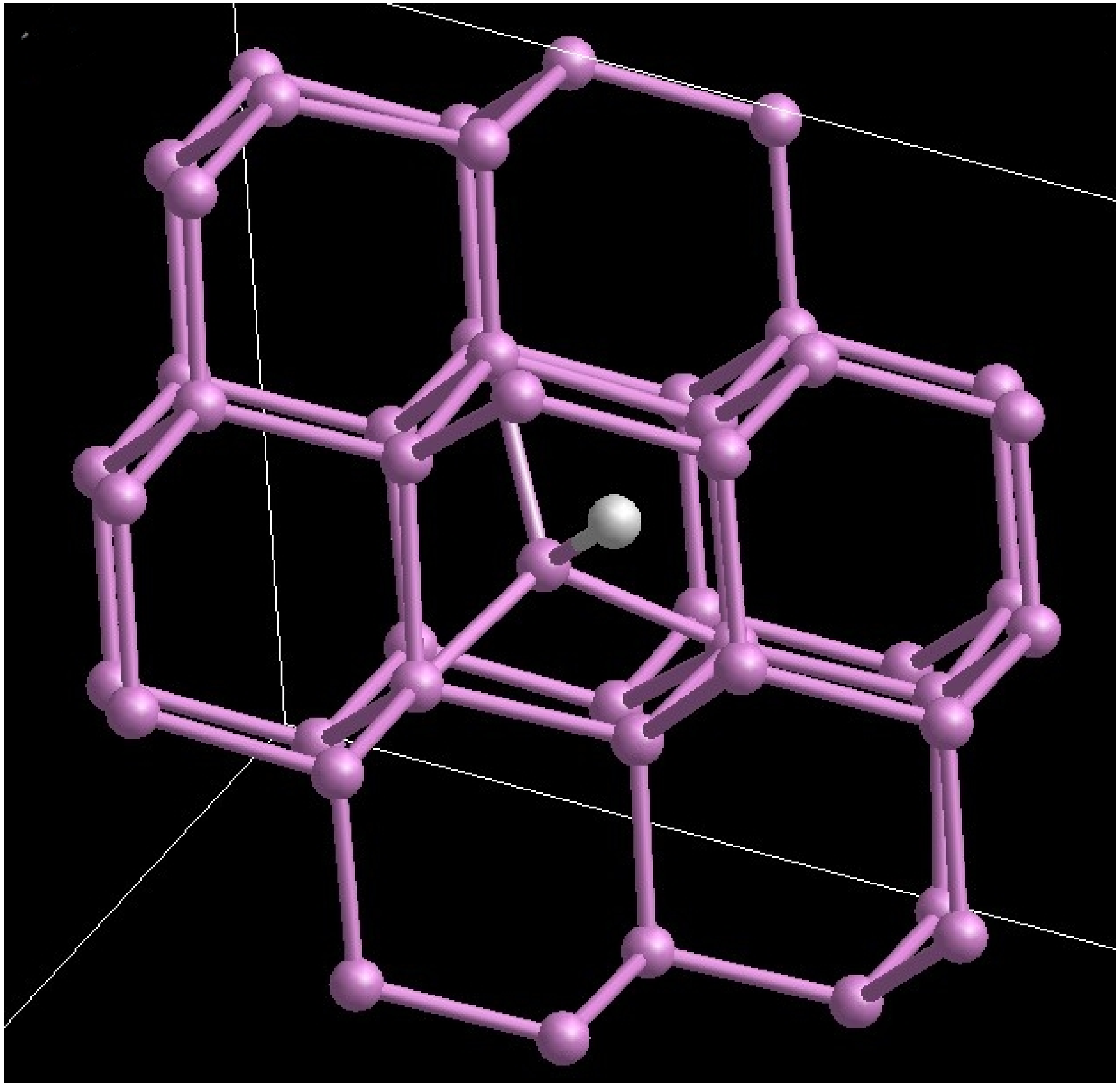
- Can use small cells

- Most recent project

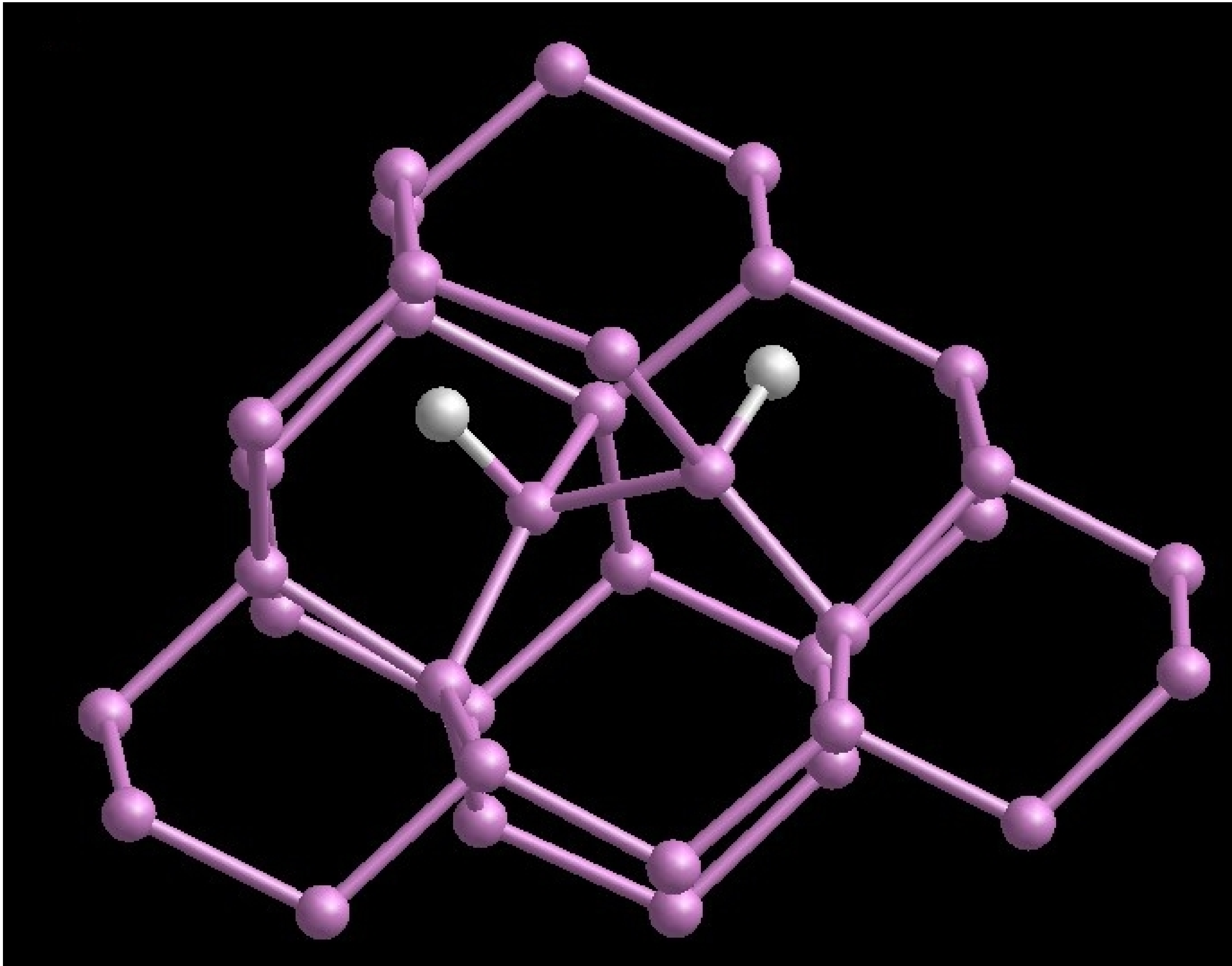
- Hydrogen changes energy states can get activation and passivation from H impurities

- Some previous studies, carried out from symmetry arguments

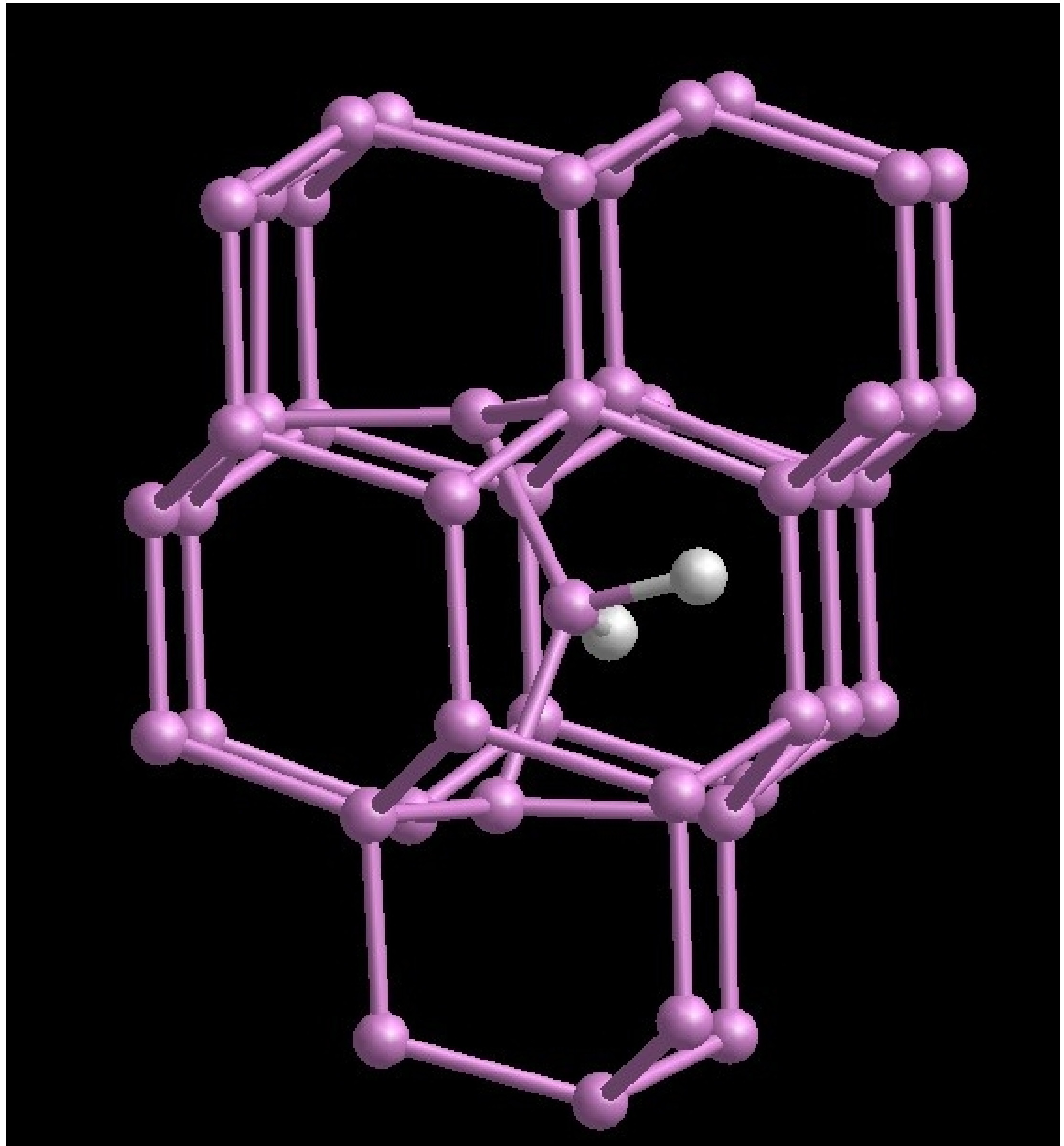
Silicon with 1 extra Silicon and 1 Hydrogen



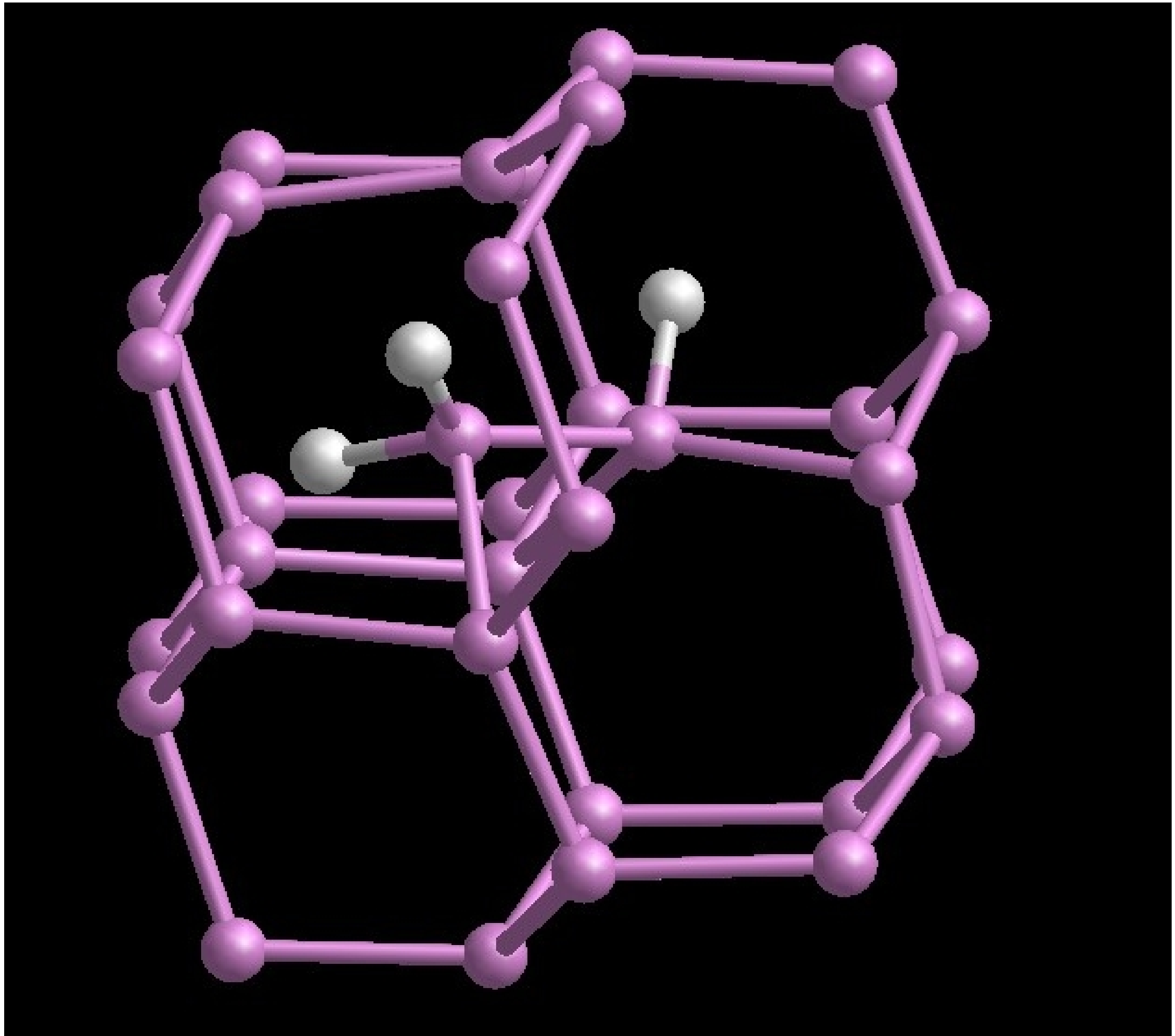
Silicon with 1 extra Silicon and 2 Hydrogen



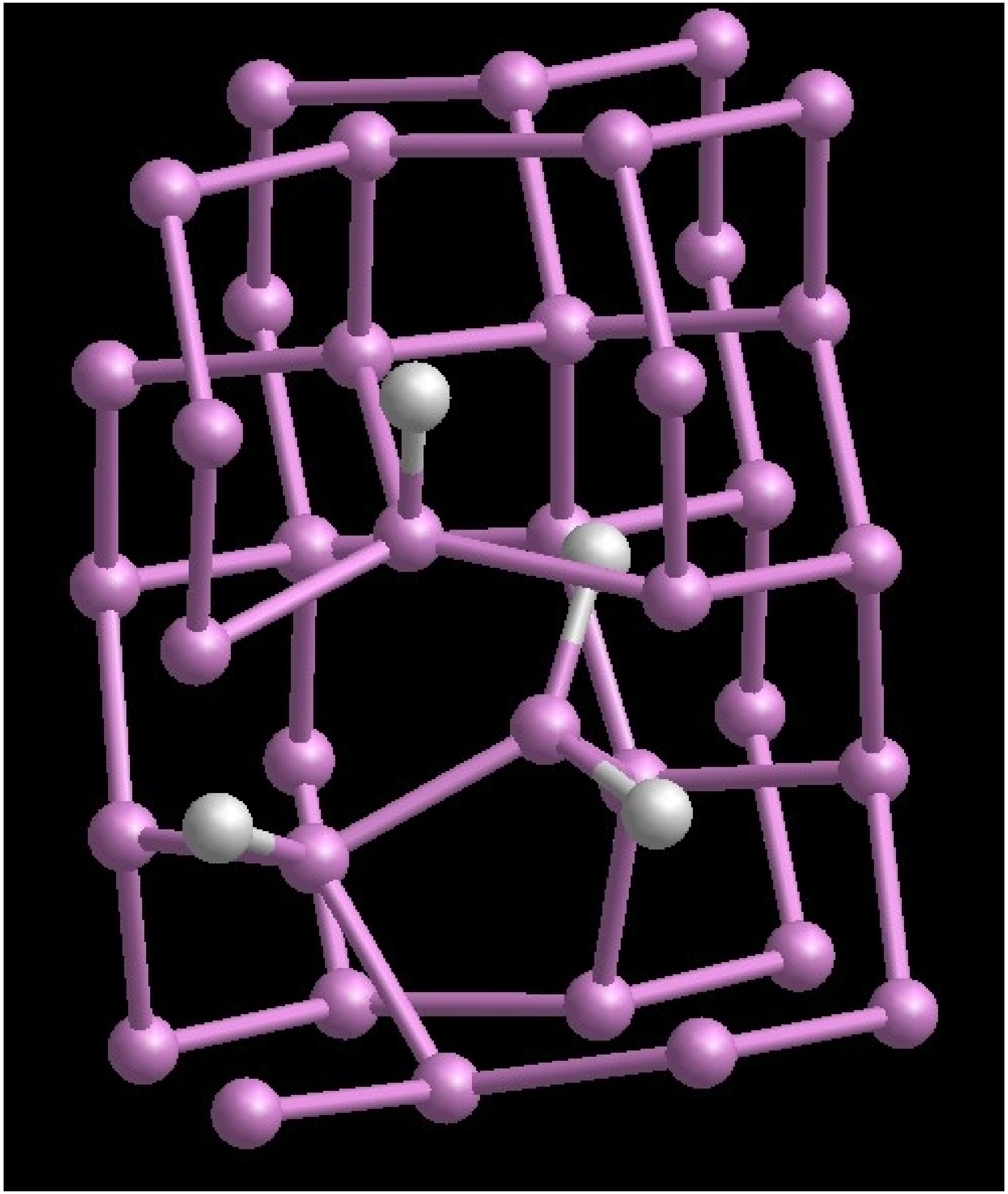
Silicon with 1 extra Silicon and 2 Hydrogen*



Silicon with 1 extra Silicon and 3 Hydrogen

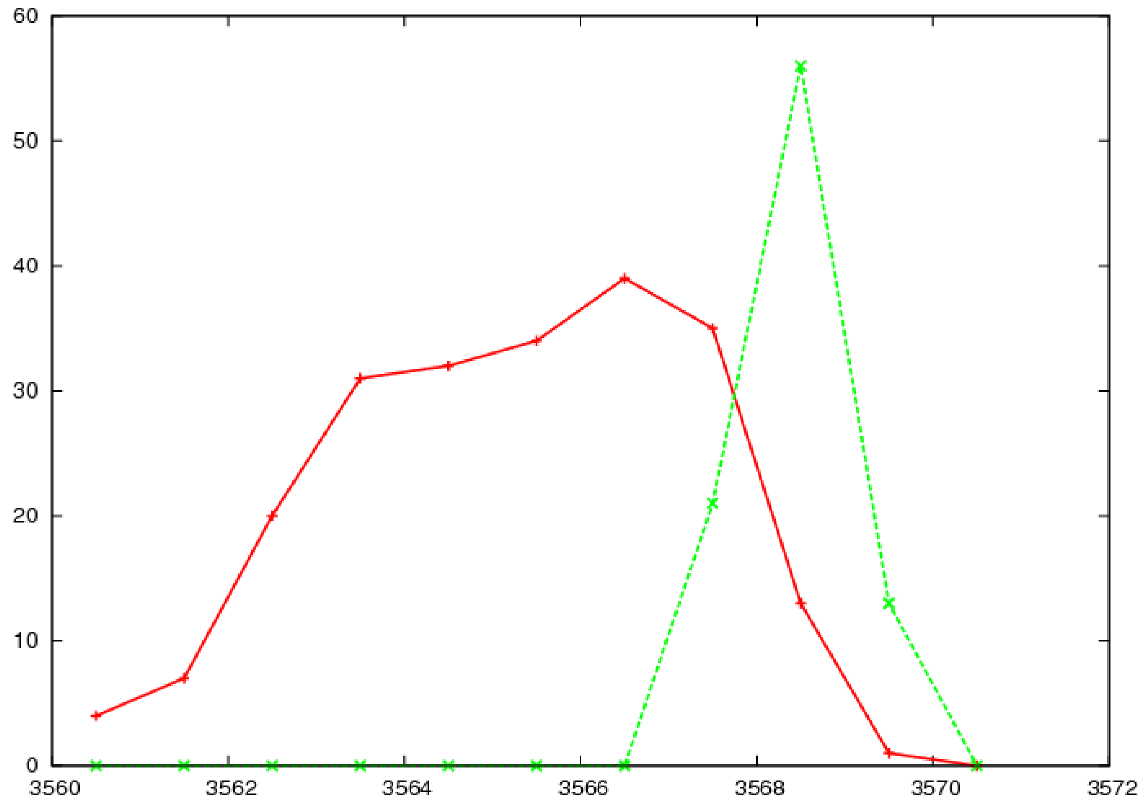


Silicon with 1 extra Silicon and 4 Hydrogen



Problems and Tweaks

- Difficult to find the I+H2 ground state from a 5 atom hole.
- Tried again from a 1 atom hole.
- Get the right I+H2 defect quite quickly.
- Have also tried 1 atom holes from hexagonal site.
- Gives some of the best results.



Conclusions

Random Structure Searching in Defects works, and can reproduce results found by other methods

We have a method now, that can generate results quickly

Fish / Polish / Embed / (Publish)

Constraints are important to reduce the search space.

Start with a small hole on a well-defined site and randomise.

The beauty of the method is in the the simplicity of the algorithm

Unlike other methods, we don't have to think up starting configs. that bias the results.

Acknowledgements

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