The 37th CMD workshop "Advanced study with ES-opt"

Synthesis simulation with DFT

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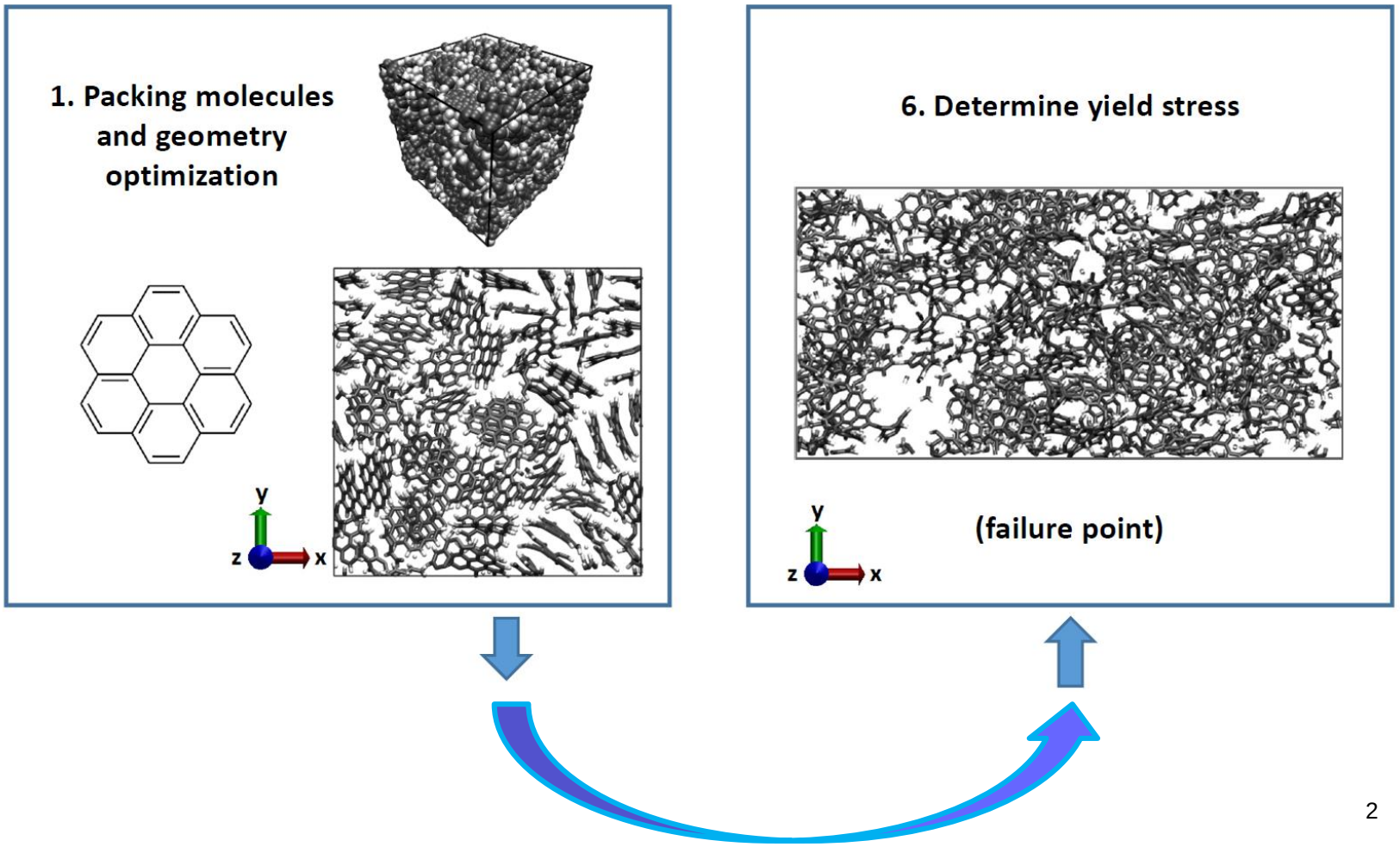
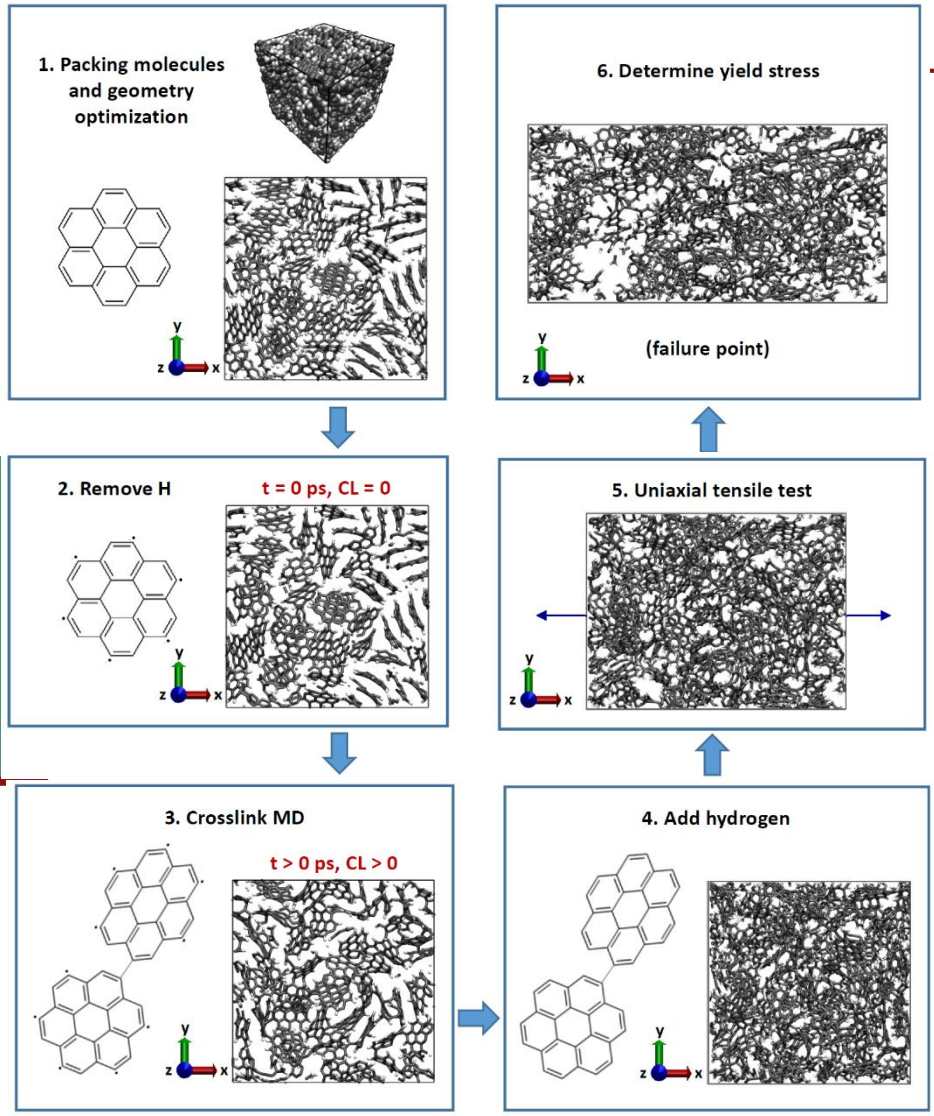
A simulation of “carbonization”



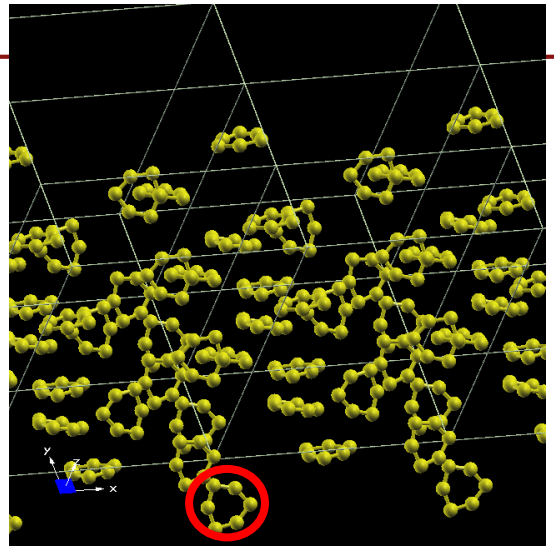
Cf. Preprint Cambridge Center for Computational Chemical Engineering ISSN 1473-4283 by L. Pascazio, et al. (18 June 2018)

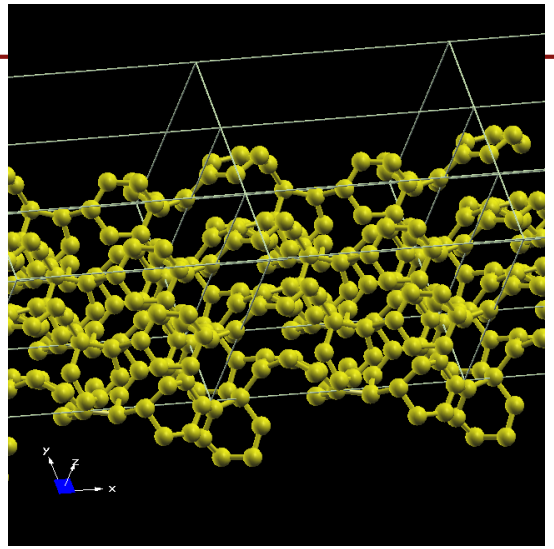


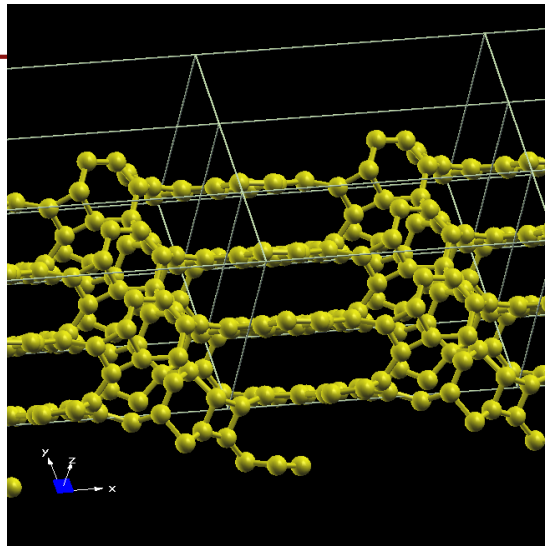
- Poly-aromatic hydro-carbon (PAH) molecules are in an initial condensed phase.
- Hydrogen atoms are once removed. (radical formation)
- Cross-links are given by MD.
- At an intermediate stage, hydrogen atoms are recovered to stop reaction.
- A tensile test obtaining a final structure is given in a simulation.

1) Production of soot is realized.
2) Nano-voids & nano-pores are formed.

A simple test for creation of graphitic carbon from C_6



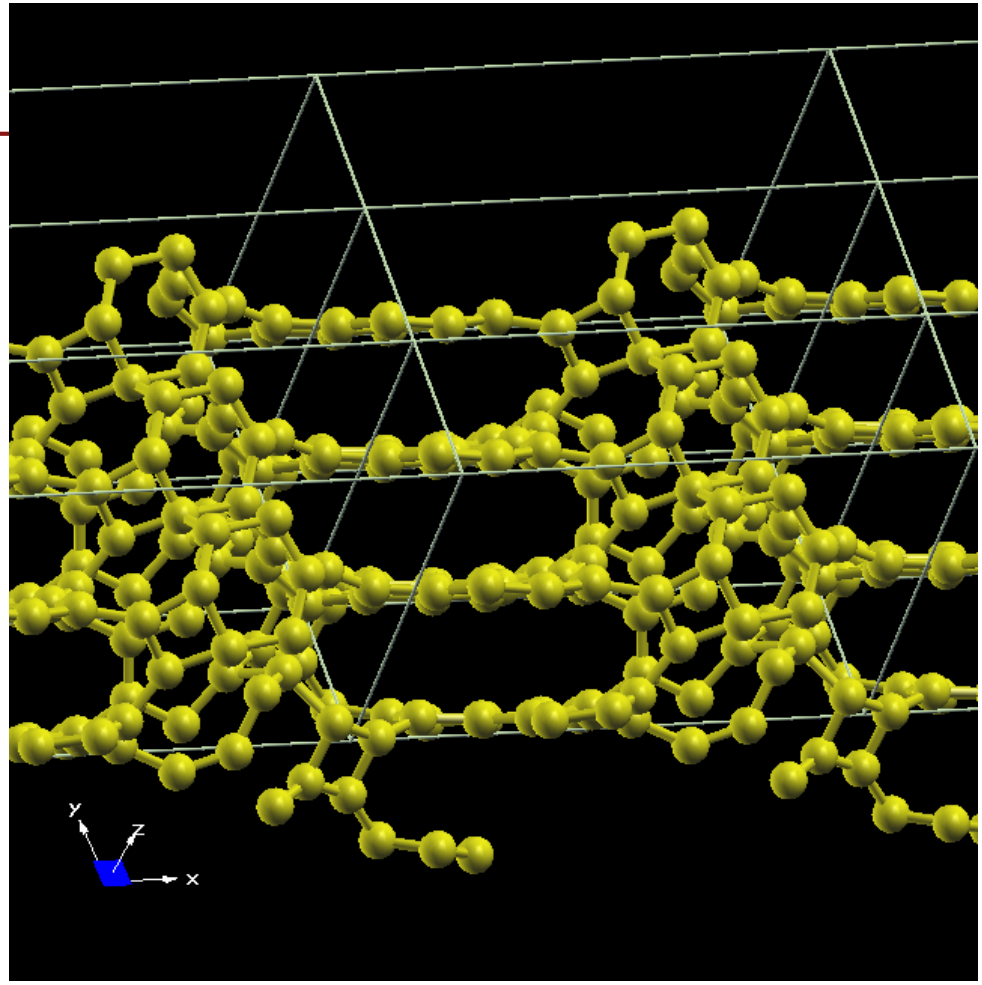


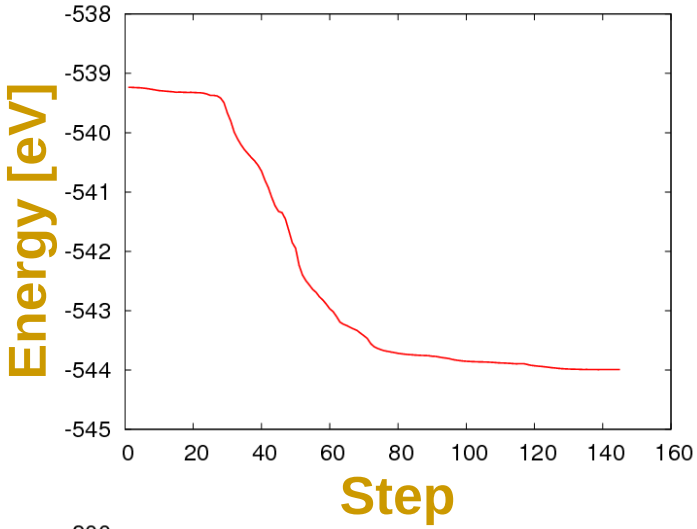


C_6 has a reduced symmetry in C_3.

6-, 5-, & 4-membered rings are created.

After optimization, we obtain graphitic form.


y
z
x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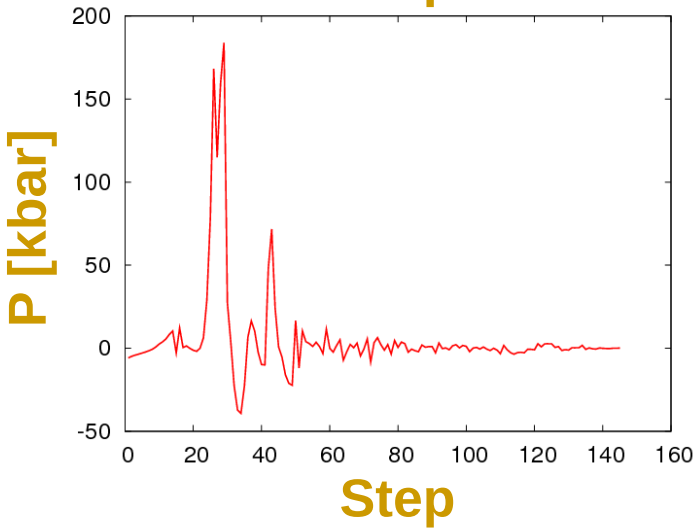
-538
-539
-540
-541
-542
-543
-544
-545
0
20
40
60
80
100
120
140
160
Step


P [kbar]
200
150
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50
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40
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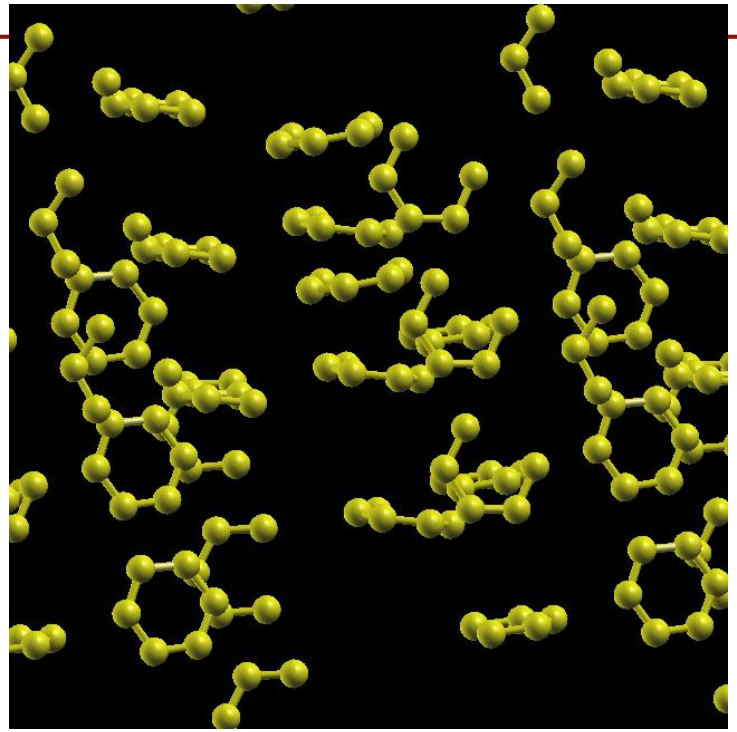
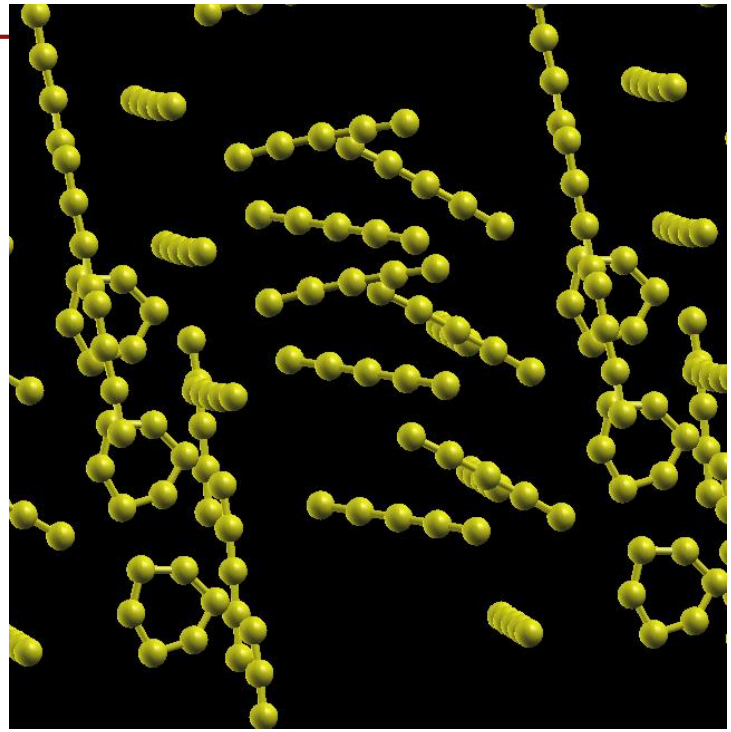
160
Step

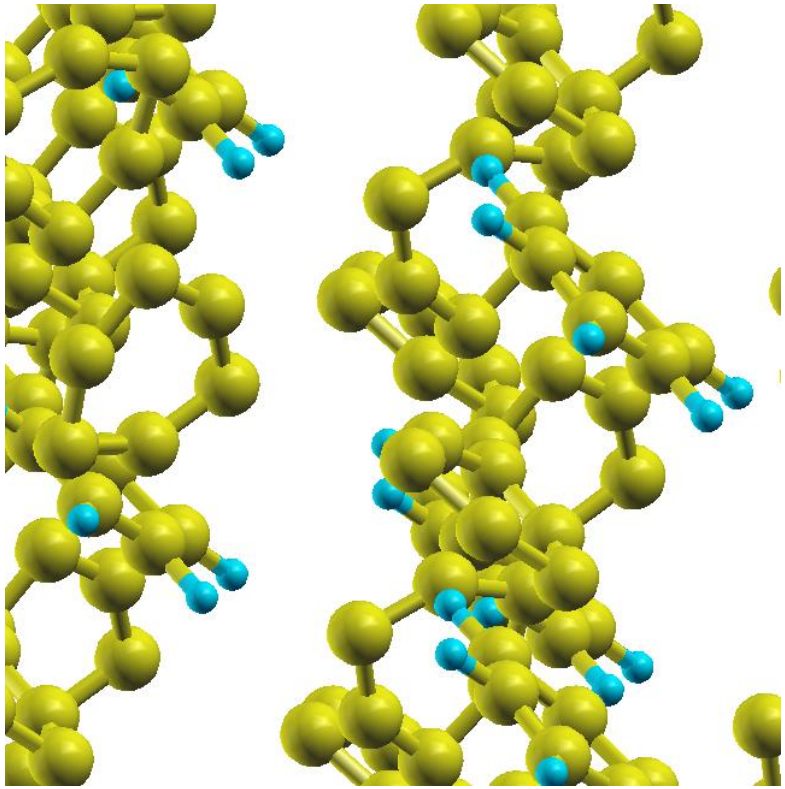


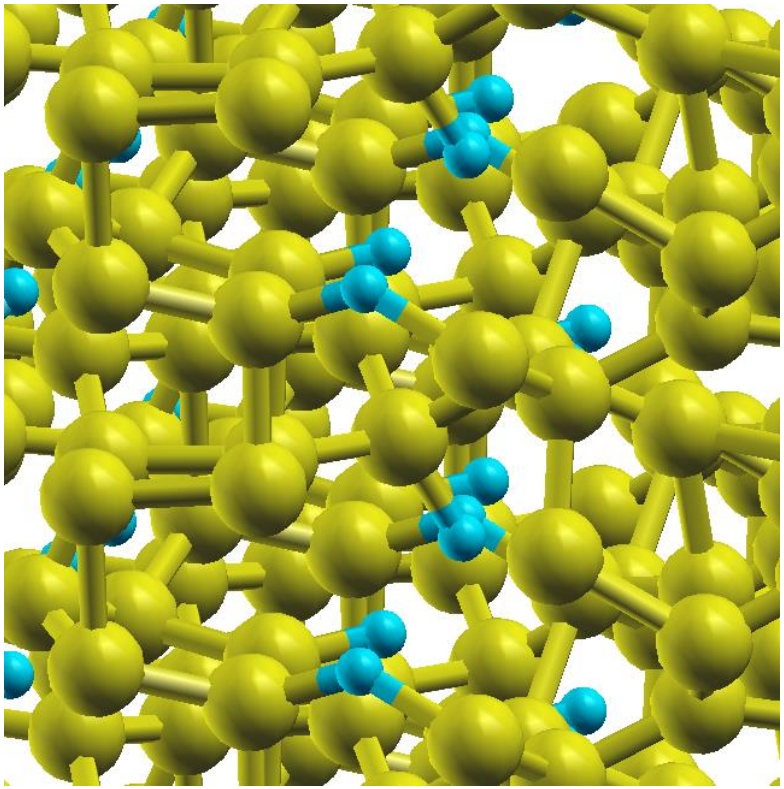
5-membered rings as defective 6-membered rings are added.



Then, chains (poly-carbene) are formed

An effect of hydrogen





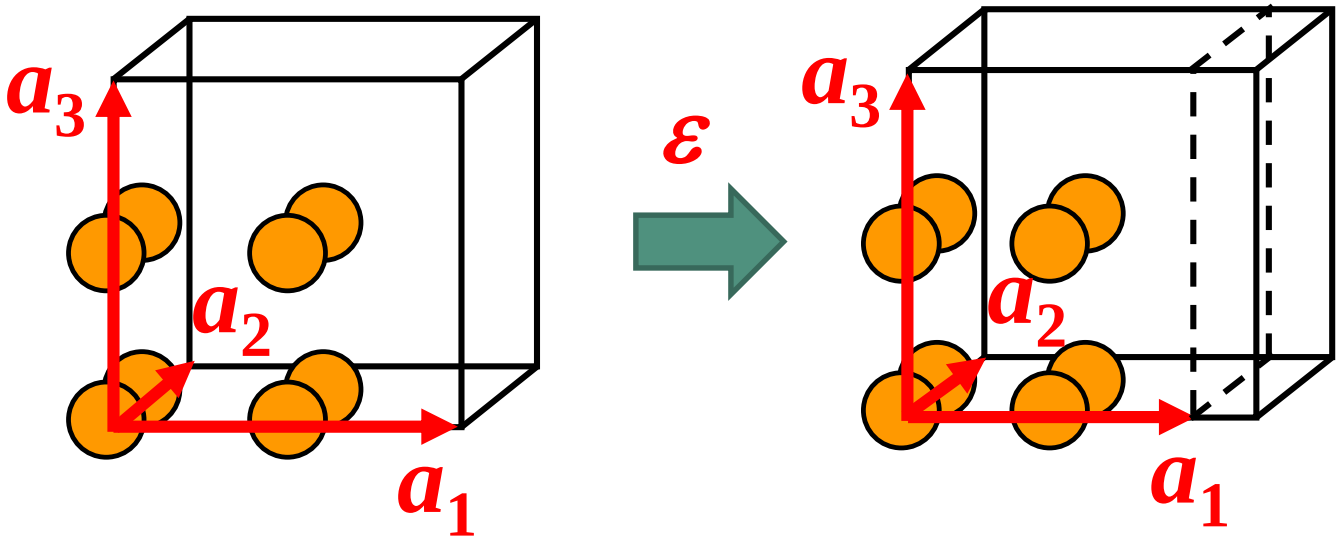
Locally diamond-like carbon appears!

An improved algorithm : EA

Genetic algorithm (遺伝的 (発生論的) アルゴリズム)
Evolutionary algorithm (進化論的アルゴリズム)

Algorithms as operations given by Oganov's group

Heredity (遺伝・世襲) **Mutation (突然変異)** **Permutation (置換)**



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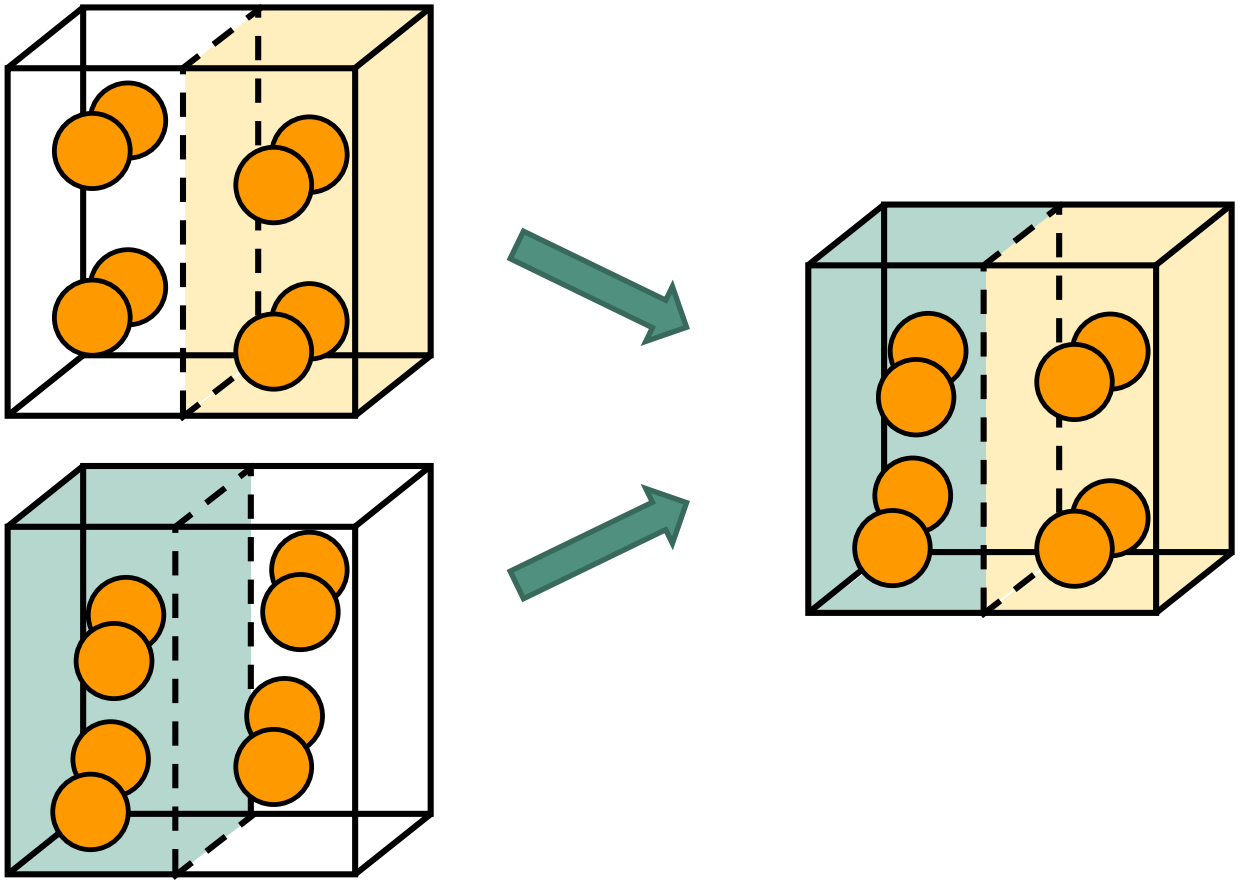

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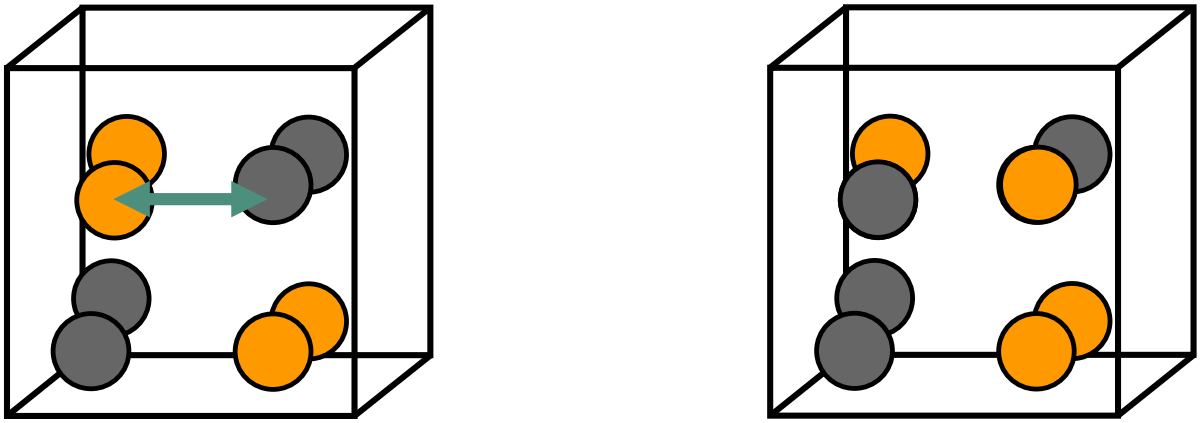

This procedure (operation) may induce “chemical reaction”.

Enhanced efficiency, acceleration in slow dynamics!