Universidad de Oviedo

POLITÉCNICA

IFN-GV

Influence of W/W grain boundaries on Helium behaviour by means of combined MD and DFT approach

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3rd Fusion HPC Workshop

Introduction

1. Why fusion? What is expected?

Future fusion Nuclear Power Plants (NPPs) are expected to provide mankind a sustainable energy source and to contribute to the energy required satisfy the growing demand of energy and to limit global warming

- Fusion offers important advantages:
  - No carbon emissions therefore, no air pollution
  - Unlimited fuel
  - Intrinsically safe

Crucial issues for reactor availability

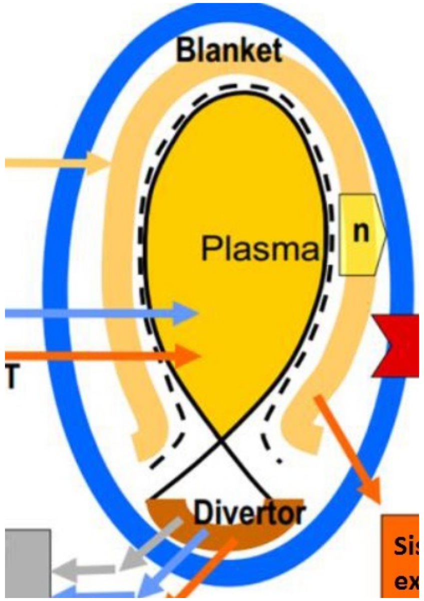
- Plasma Facing Materials (SDG7)

Introduction

Plasma facing materials are those directly exposed to:

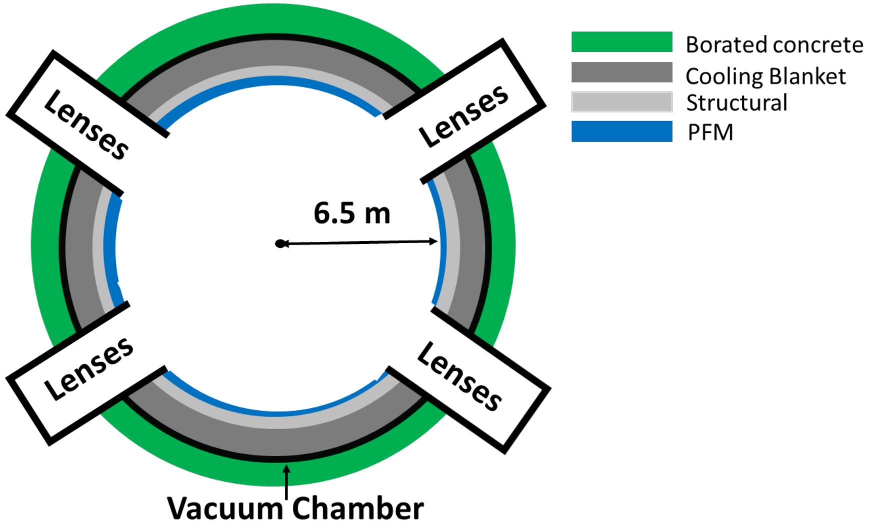
- The plasma in magnetic fusion (PFM)
- To the explosion threats in inertial fusion confinement (PFM or FW)

MCF



ICF

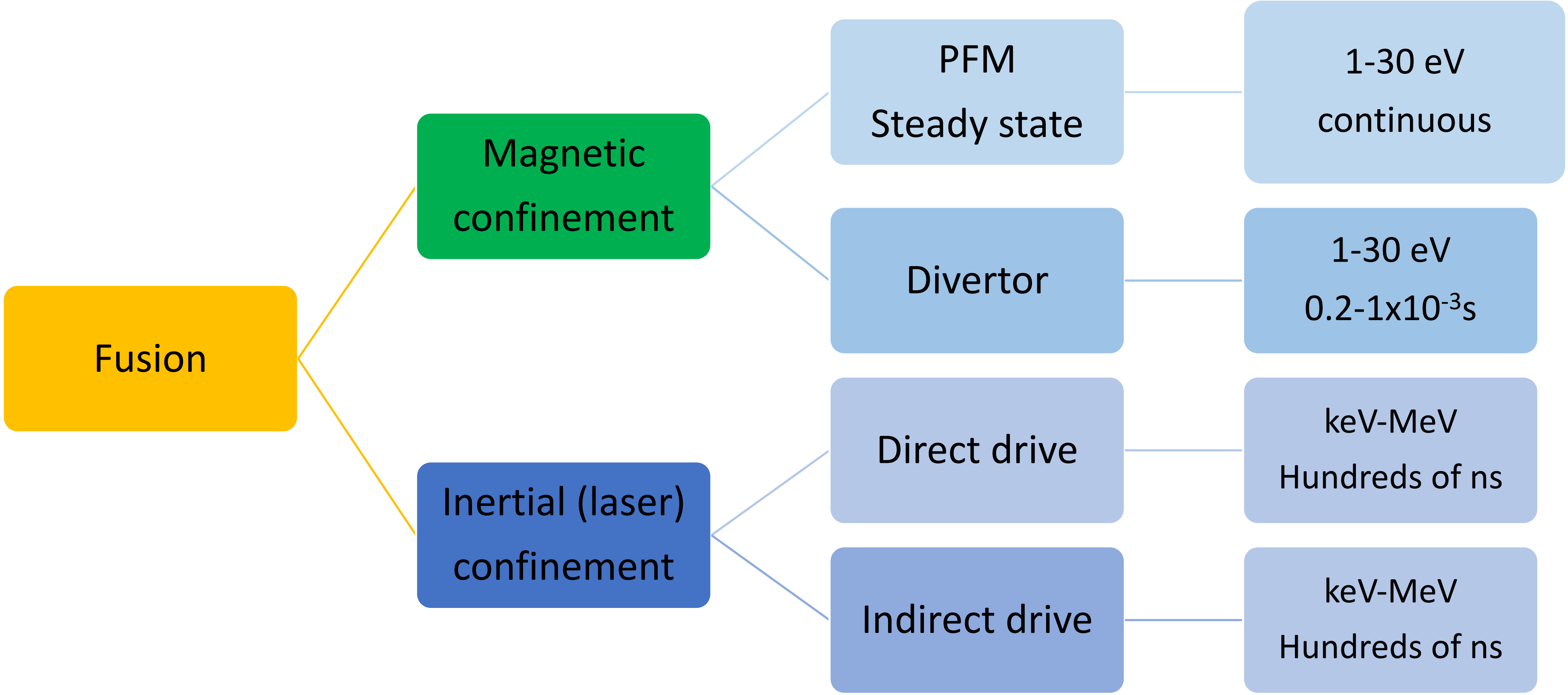
HiPER Prototype/Demo



Assignment: protect the structural materials located underneath

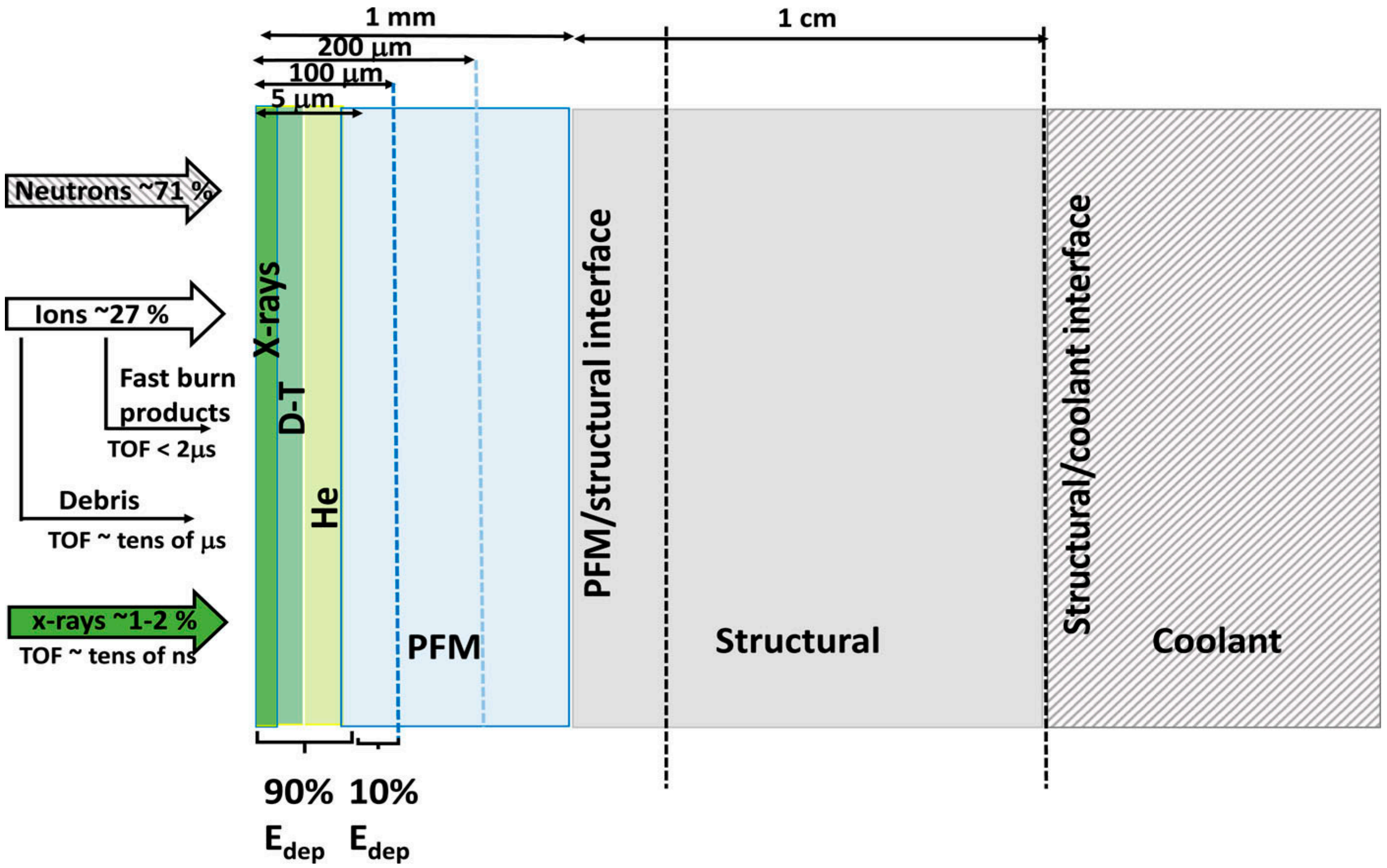
Introduction

- The main threats depend on the radiation conditions → reactor configuration



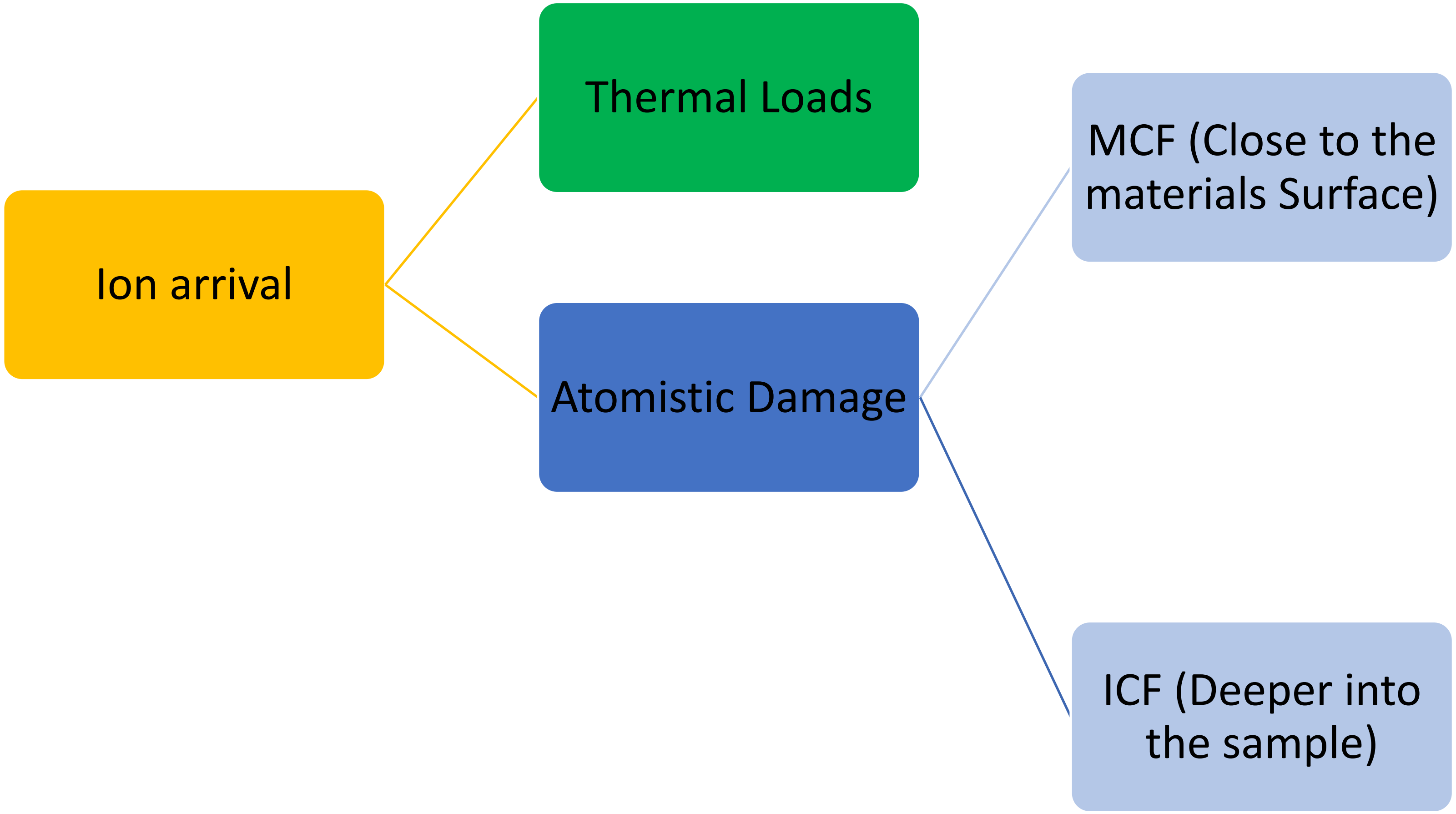
Neutrons are not real threats

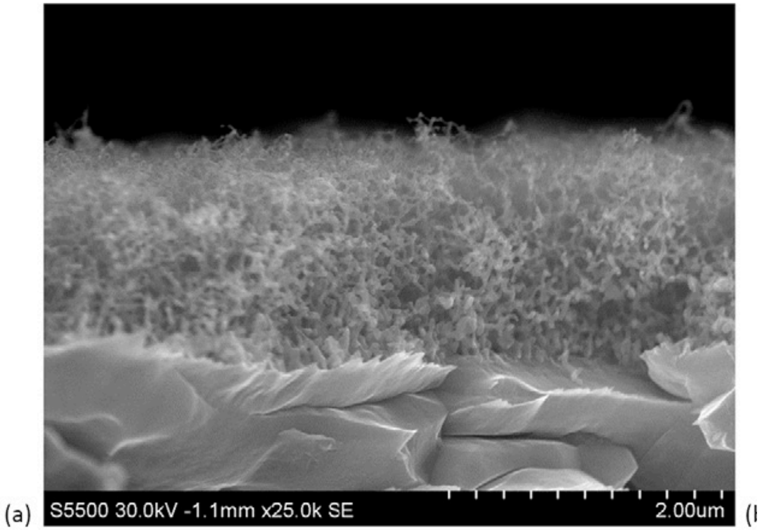
Introduction

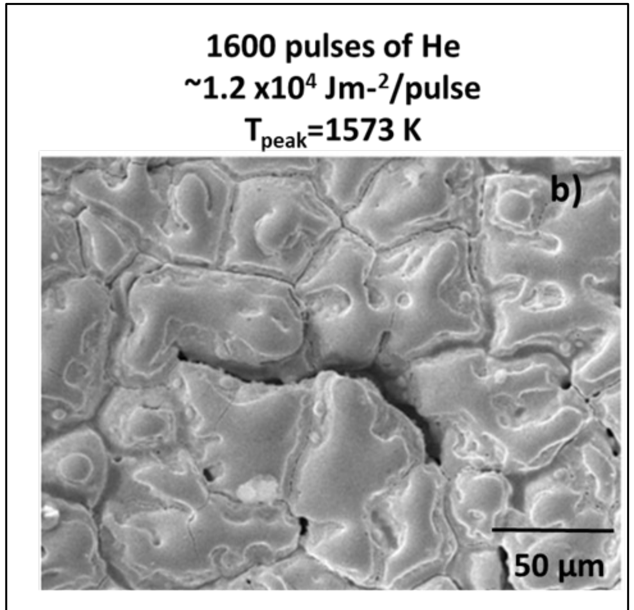


Published in: R. Gonzalez-Arrabal; A. Rivera; J. M. Perlado; *Matter and Radiation at Extremes* **5,** 055201 (2020)
DOI: 10.1063/5.0010954

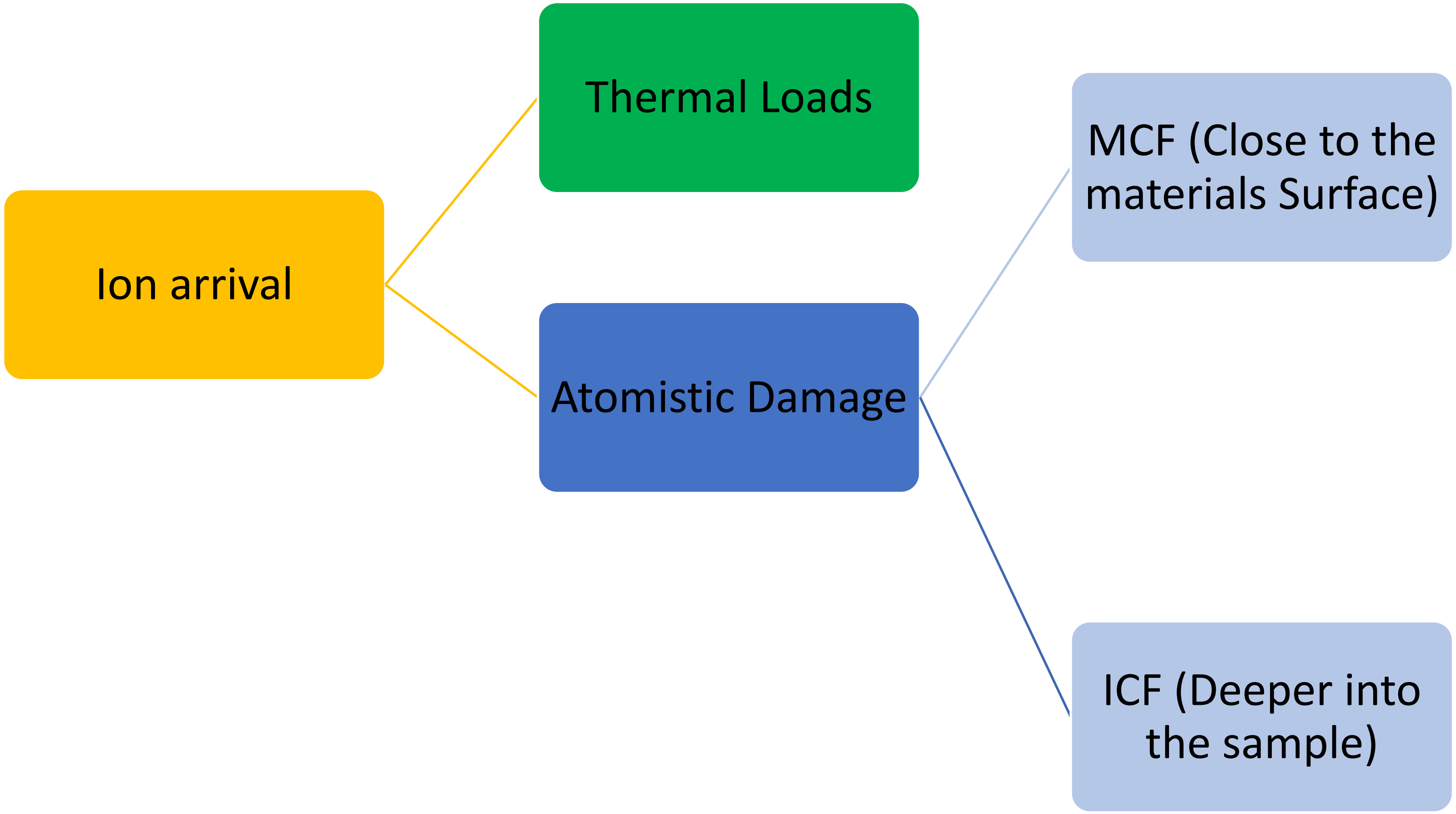
Introduction

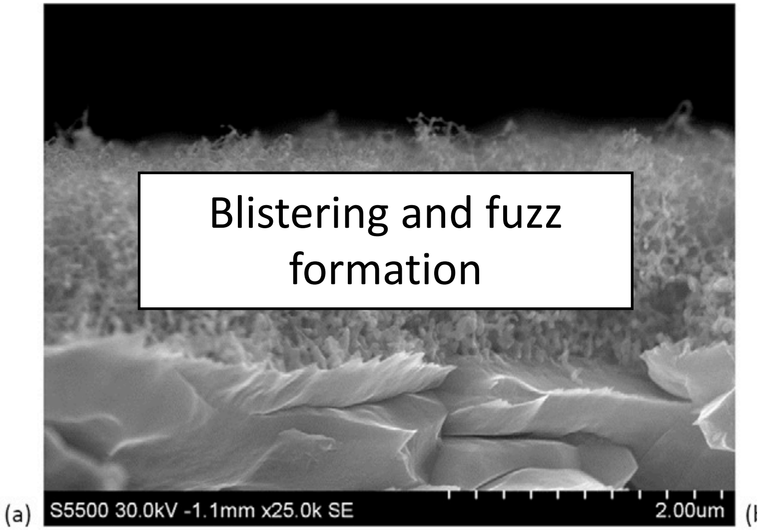


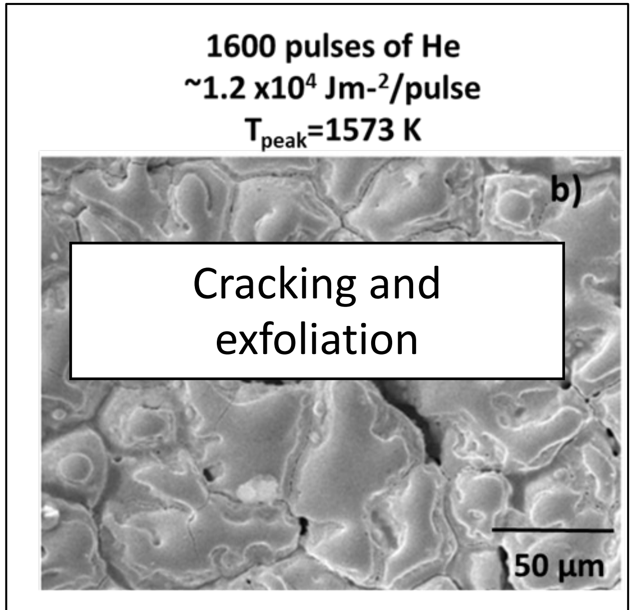




Introduction







PFM: requirements

The main requirements that must be met are summarized in:

- Good structural stability always have to be there
- Highly resistant thermal shocks
- High thermal conductivity
- High melting point
- Low physical and chemical sputtering
- Compatibility with the refrigerant
- Low retention of Tritium

PFM: candidates

- W (coarse grained W) used to be the most promising one

- Other candidates:
  - Be (low melting point, T_m~ 1287 ºC) ✗
  - Carbon fibre composites (CFCs) ✗
    - Good thermal conductivity (similar to that of Cu), but it strongly degrades in the presence of irradiation
    - Tritium retention $\rightarrow$ licensing problems

PFM: candidates

- W (coarse grained W) used to be the most promising one

- Low sputtering yields ✅
- High thermal conductivity (174 W/Km) ✅
- High melting point (3410 ºC) ✅

PFM: candidates

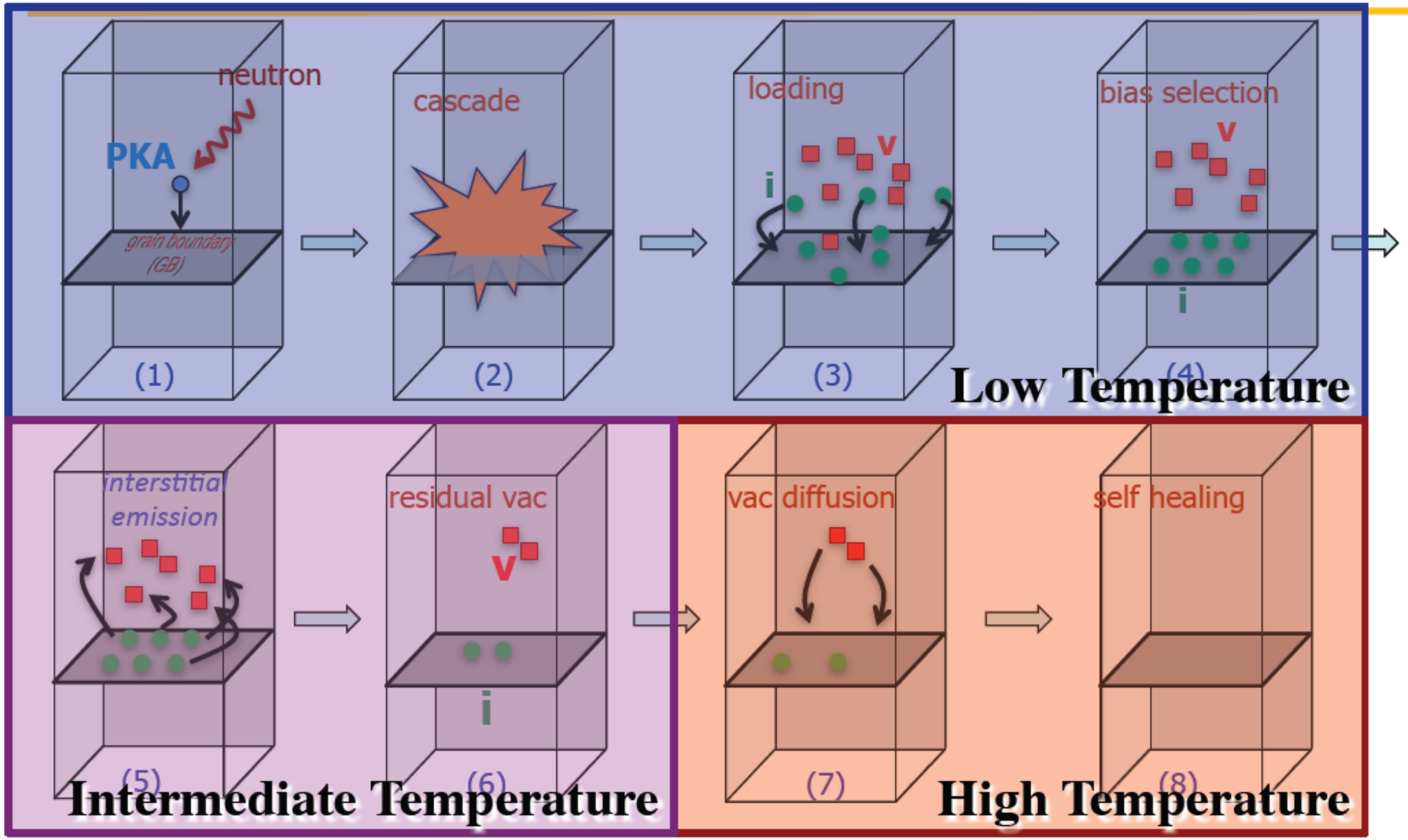
- W (coarse grained W) used to be the most promising one

- Low sputtering yields ✅
- High thermal conductivity (174 W/Km) ✅
- High melting point (3410 ºC) ✅

- Oxidation at elevated temperatures ✘
- Low recrystallization temperature () ✘
- High ductile-brittle transition temperature (423-673 K) ✘
- Low elastic limit ✘
- **High capacity to retain light species (He and H)** ✘

PFM: alternatives (W nanostructured)

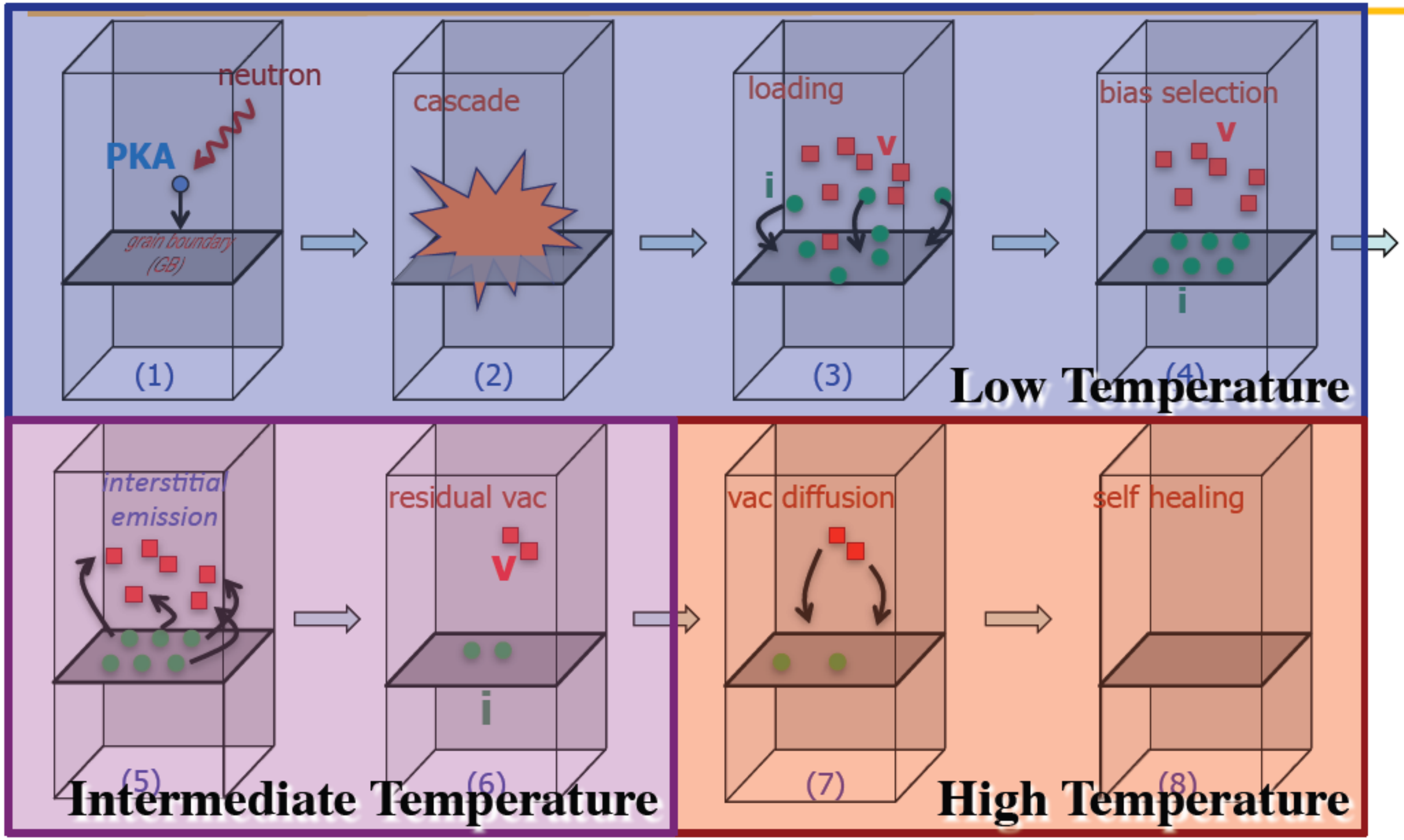
- Self-healing ✅
- Delay the pressurized bubble formation ✅



I. J. Beyerlein *et al.* Materials Today 16 (2013) 443–449.

PFM: alternatives (W nanostructured)

- Self-healing ✅
- Delay the pressurized bubble formation ✅
- He! ❌

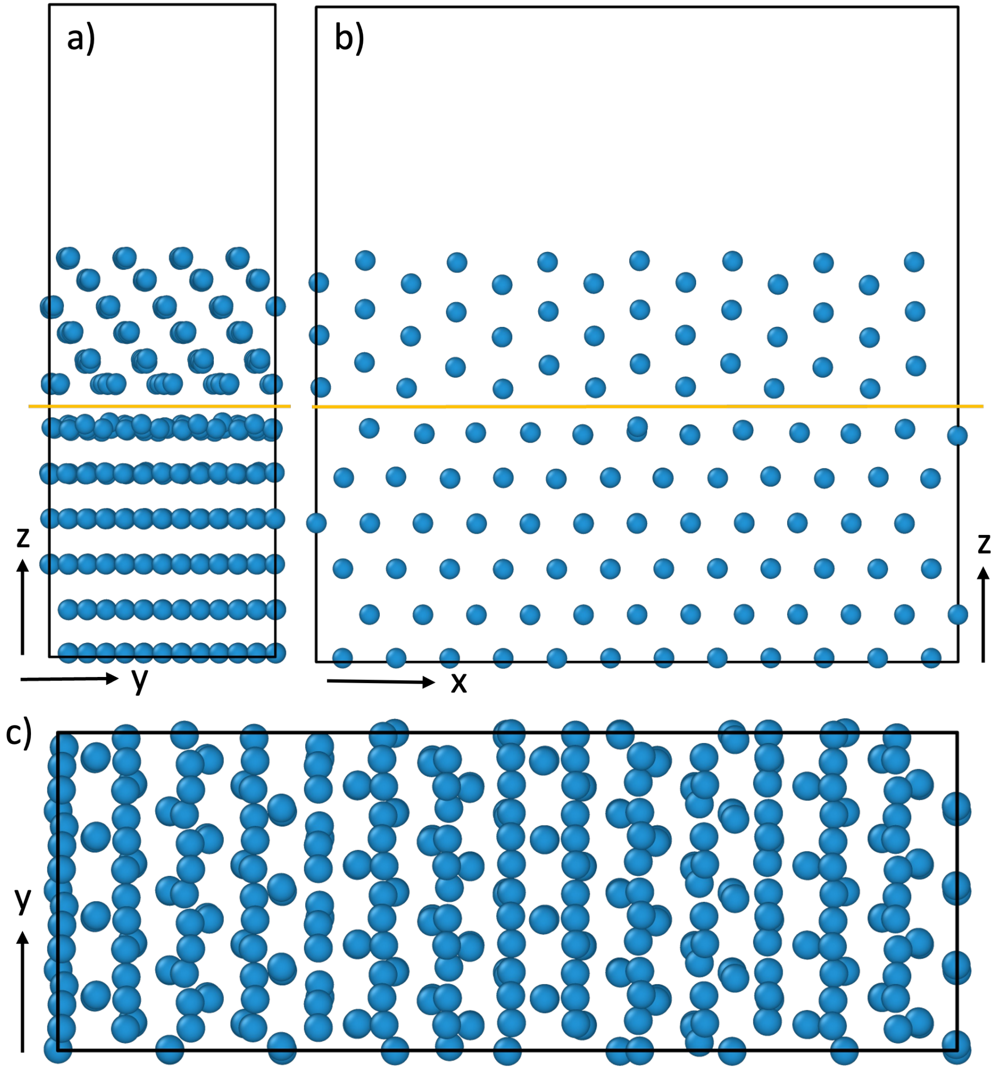


I. J. Beyerlein *et al.* Materials Today 16 (2013) 443–449.

W(110) / W(112) Interface

W(110) / W(112) interface

- 456 atoms



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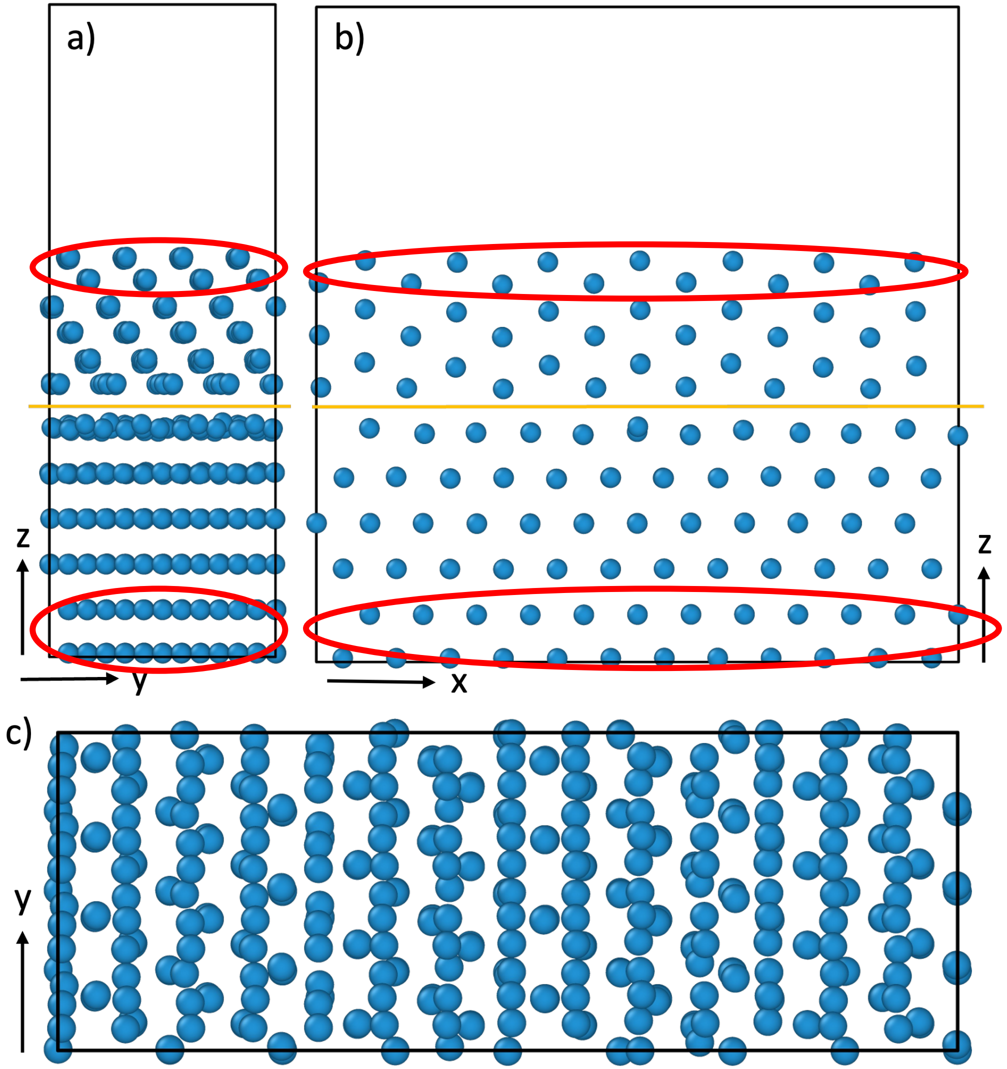

Methodology

DFT:

- Accuracy ✅
- High computational cost ❌
- Limited few hundred atoms ❌
- NO temperature ❌

CONVERGENCE PROBLEM!

Methodology

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- Accuracy ✅
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CONVERGENCE PROBLEM!

MD:

- Large system and long times ✅
- Several orders magnitude faster than DFT ✅
- Apply temperature ✅
- Interatomic Potential ❌

Methodology

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CONVERGENCE PROBLEM!

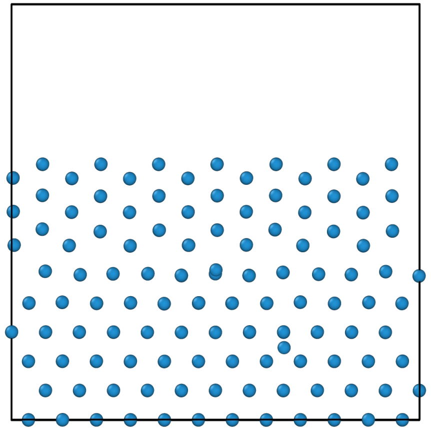
MD:

- Large system and long times ✅
- Several orders magnitude faster than DFT ✅
- Apply temperature ✅
- Interatomic Potential ❌

- Improve starting point
- Run MD bigger systems with temperature

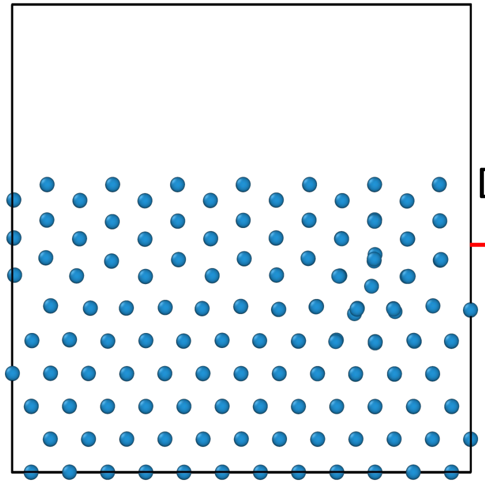
Results

Initial Configuration

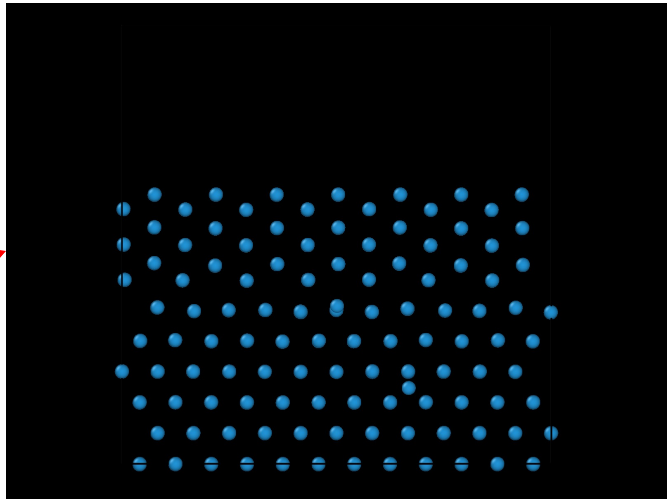


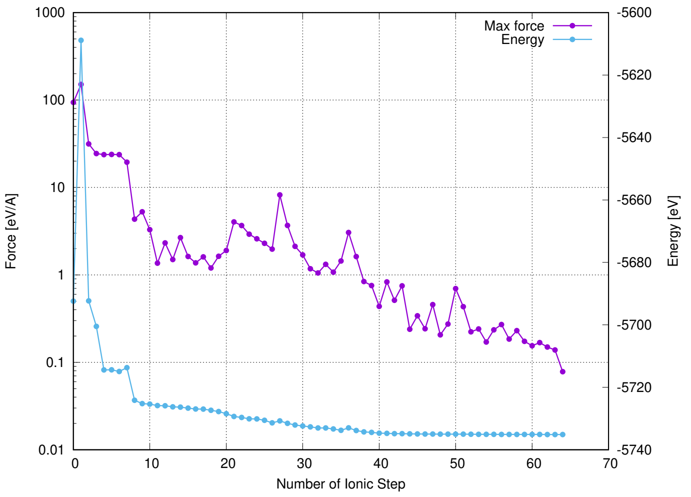
Directly DFT

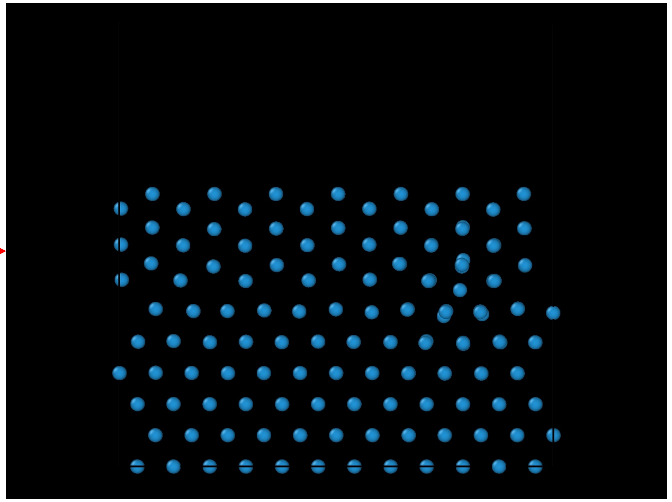
MD relaxation

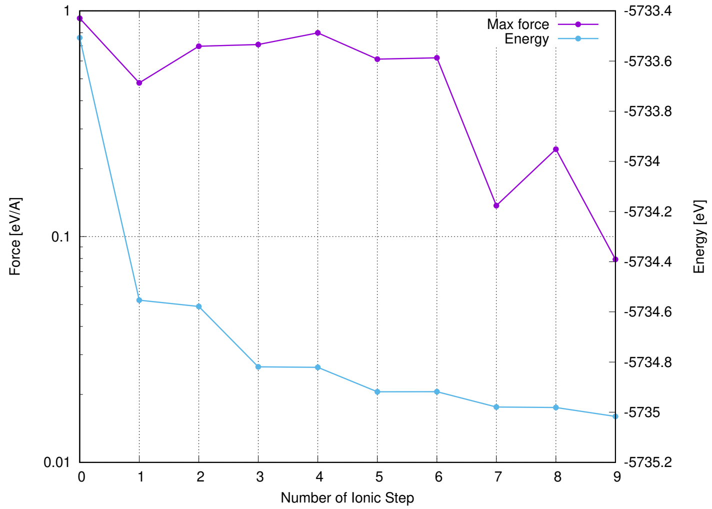


DFT



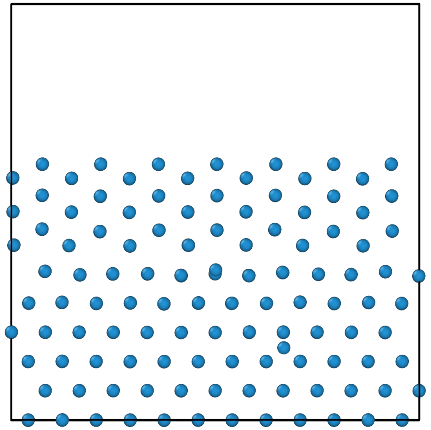




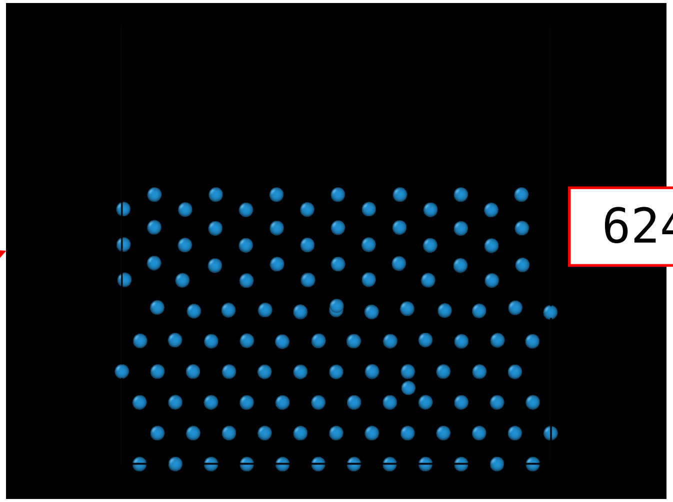


Results

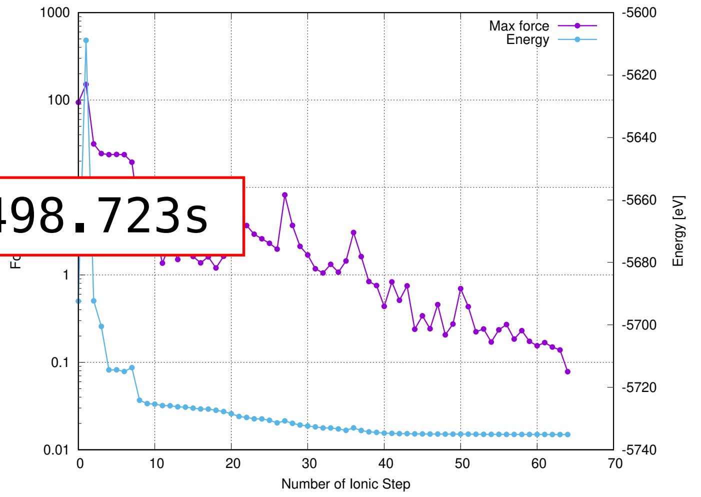
Initial Configuration



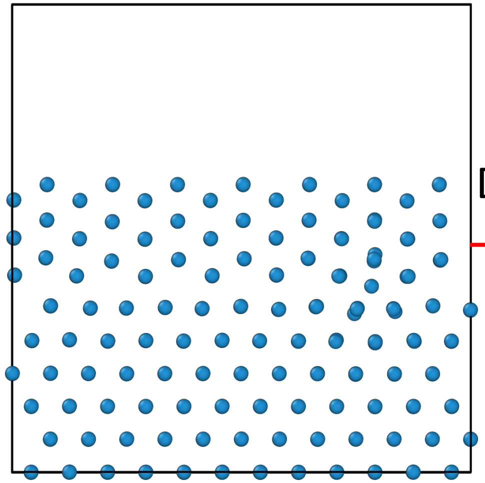
Directly DFT



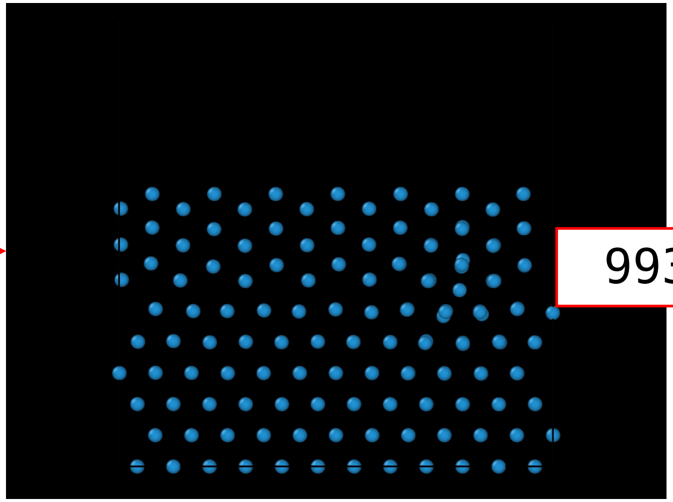
62498.723s



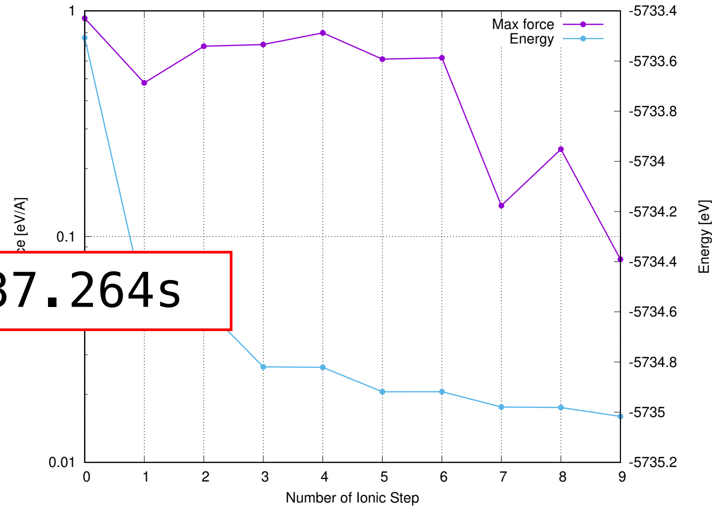
MD relaxation



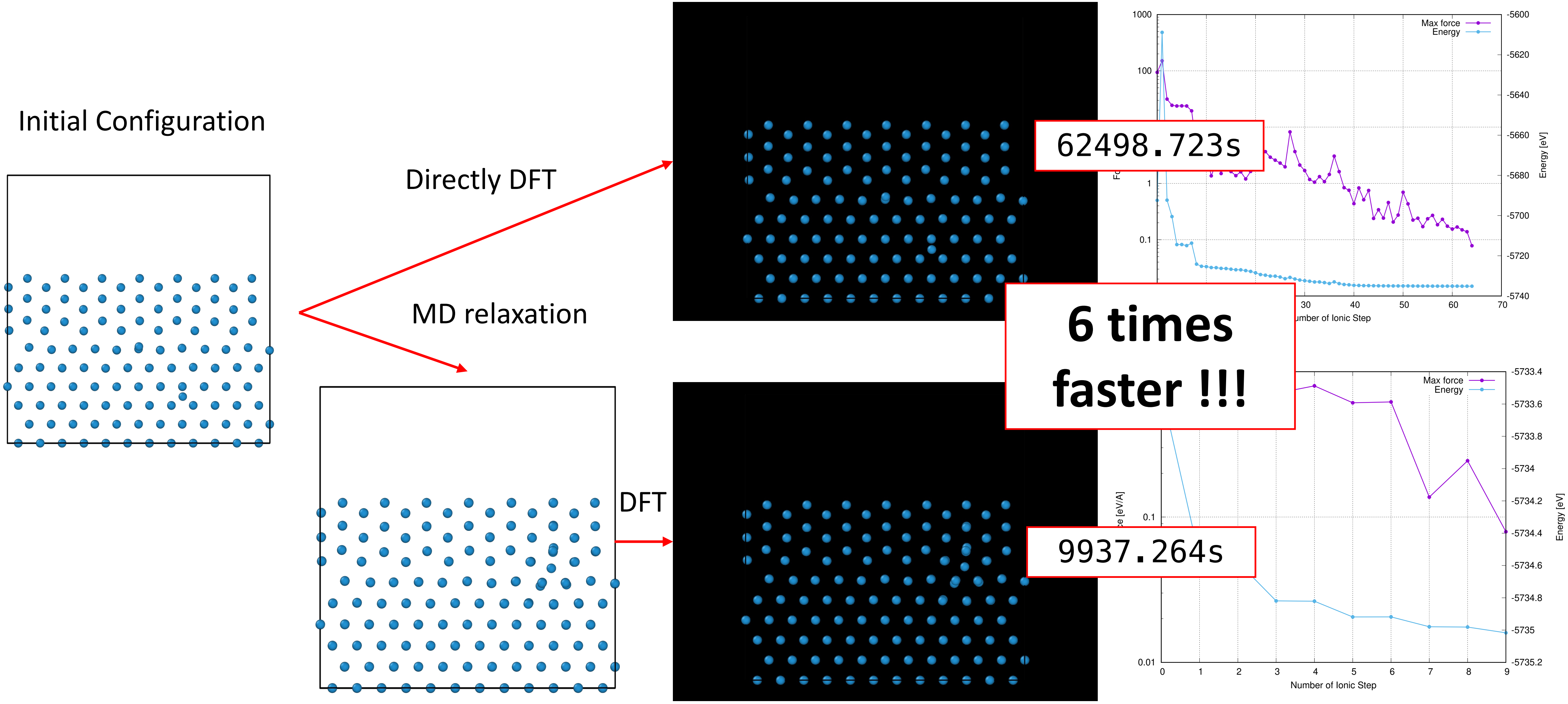
DFT



9937.264s



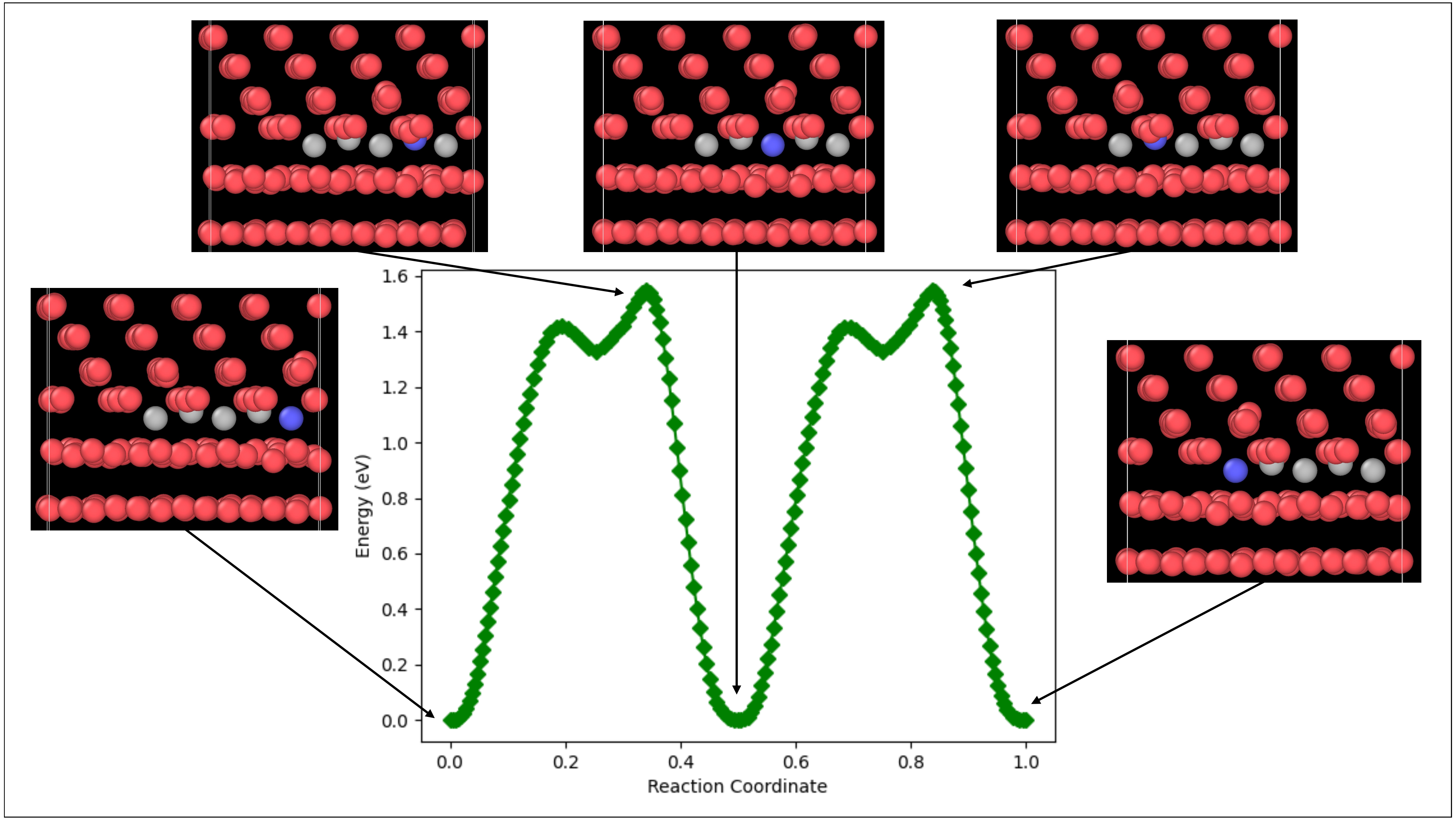
Results


Initial Configuration
Directly DFT
MD relaxation
DFT
62498.723s
6 times faster !!!
9937.264s
Max force
Energy
Energy [eV]
Number of Ionic Step

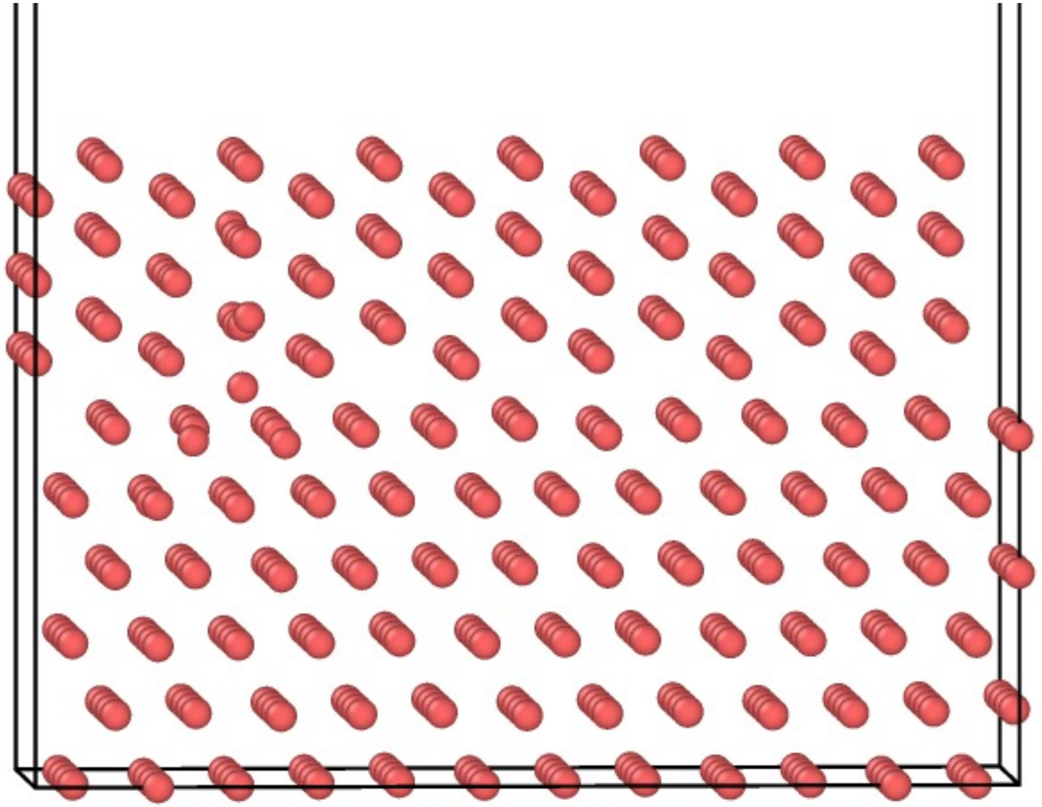
Results

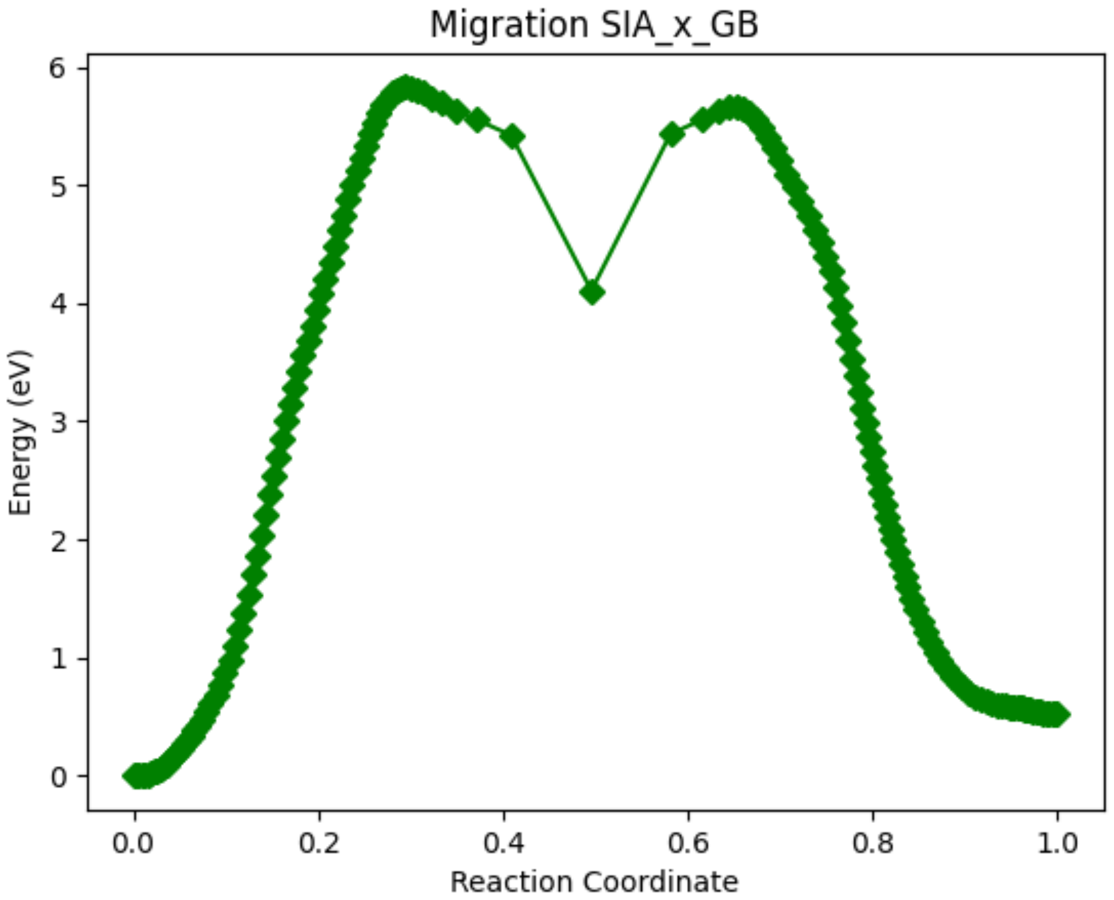
Migration Barriers

- Nudged Elastic Band (NEB)



Results

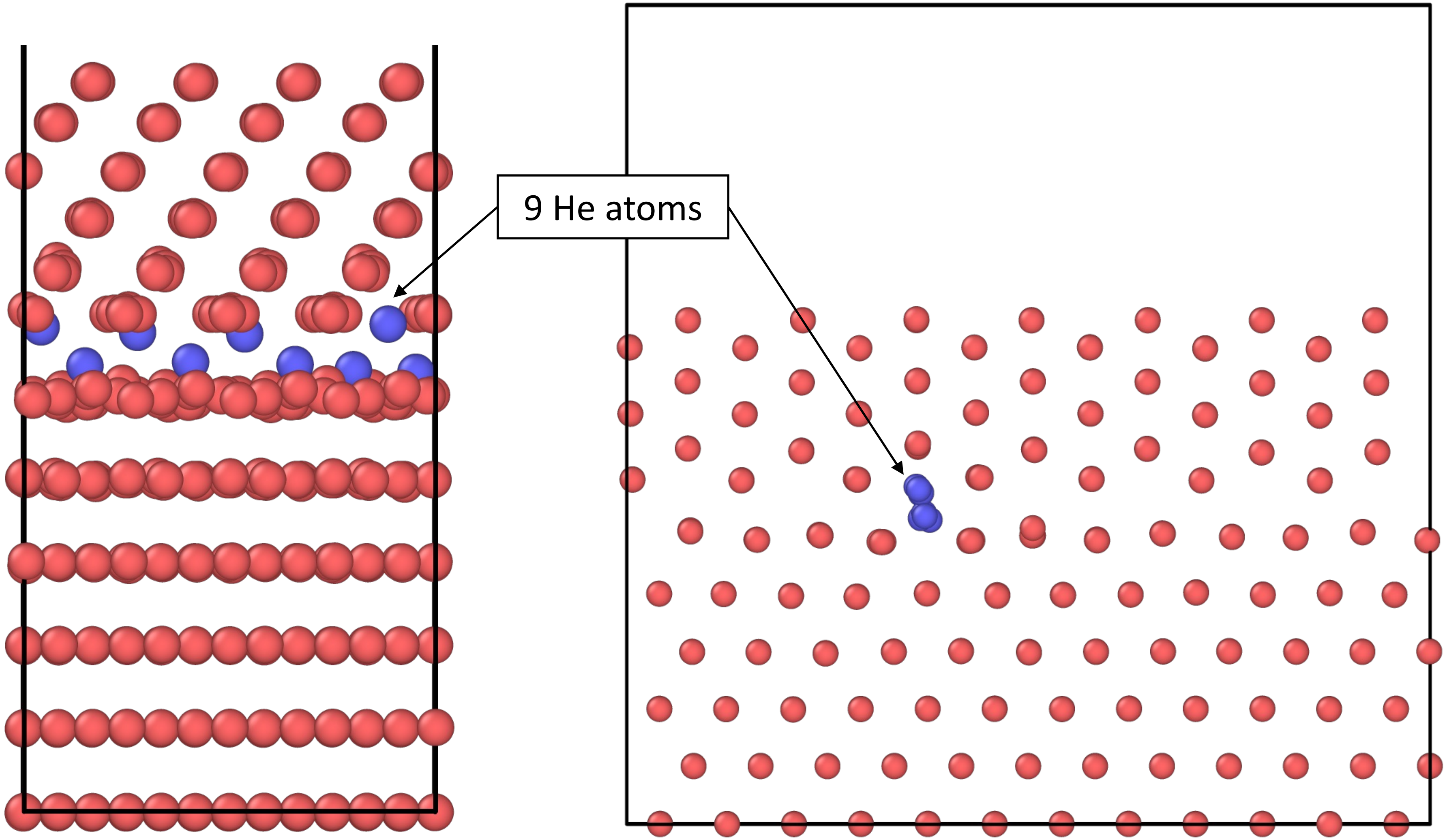




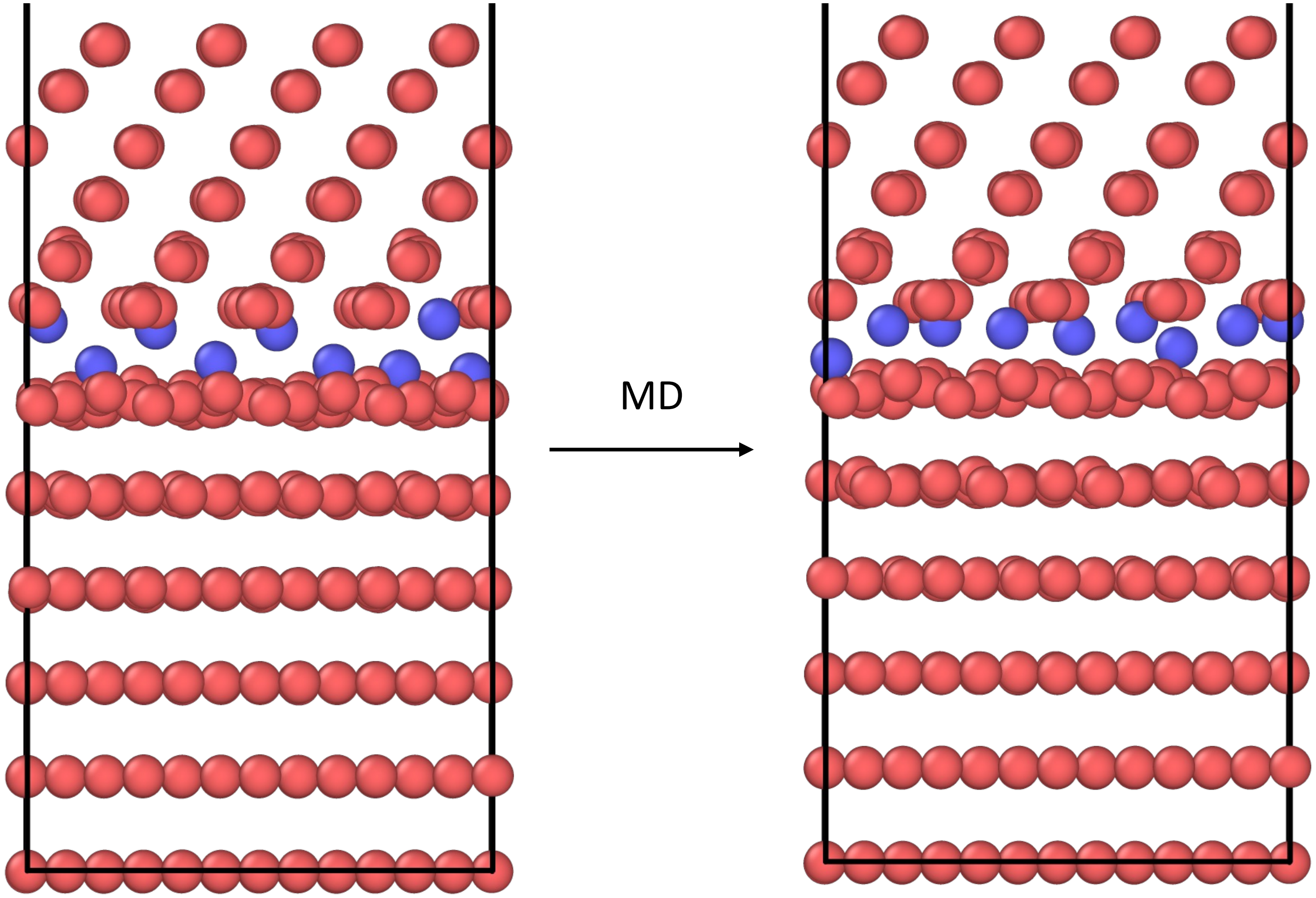
Migration SIA_x_GB
Energy (eV)
Reaction Coordinate
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0

Results

DFT



Results



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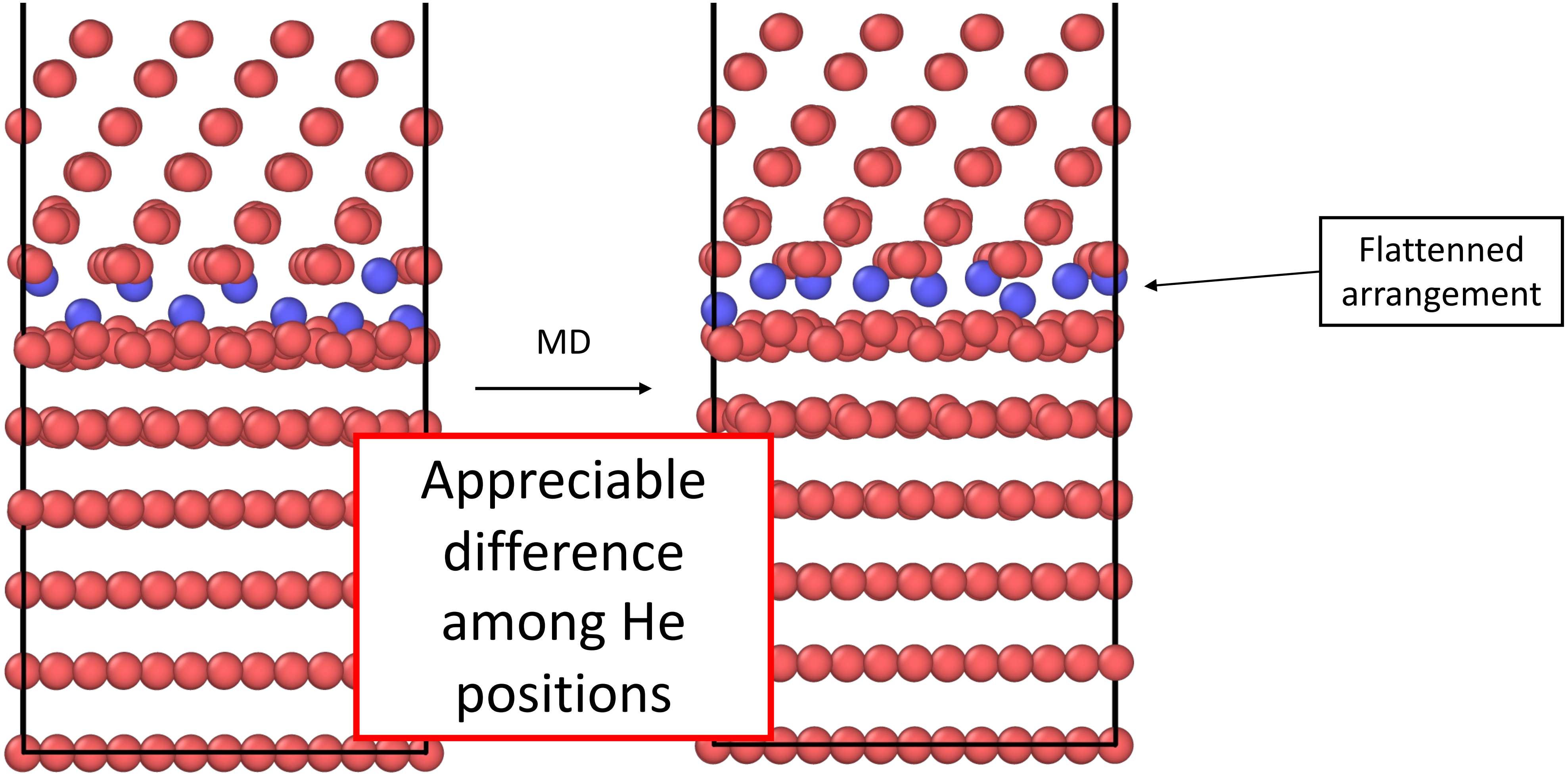
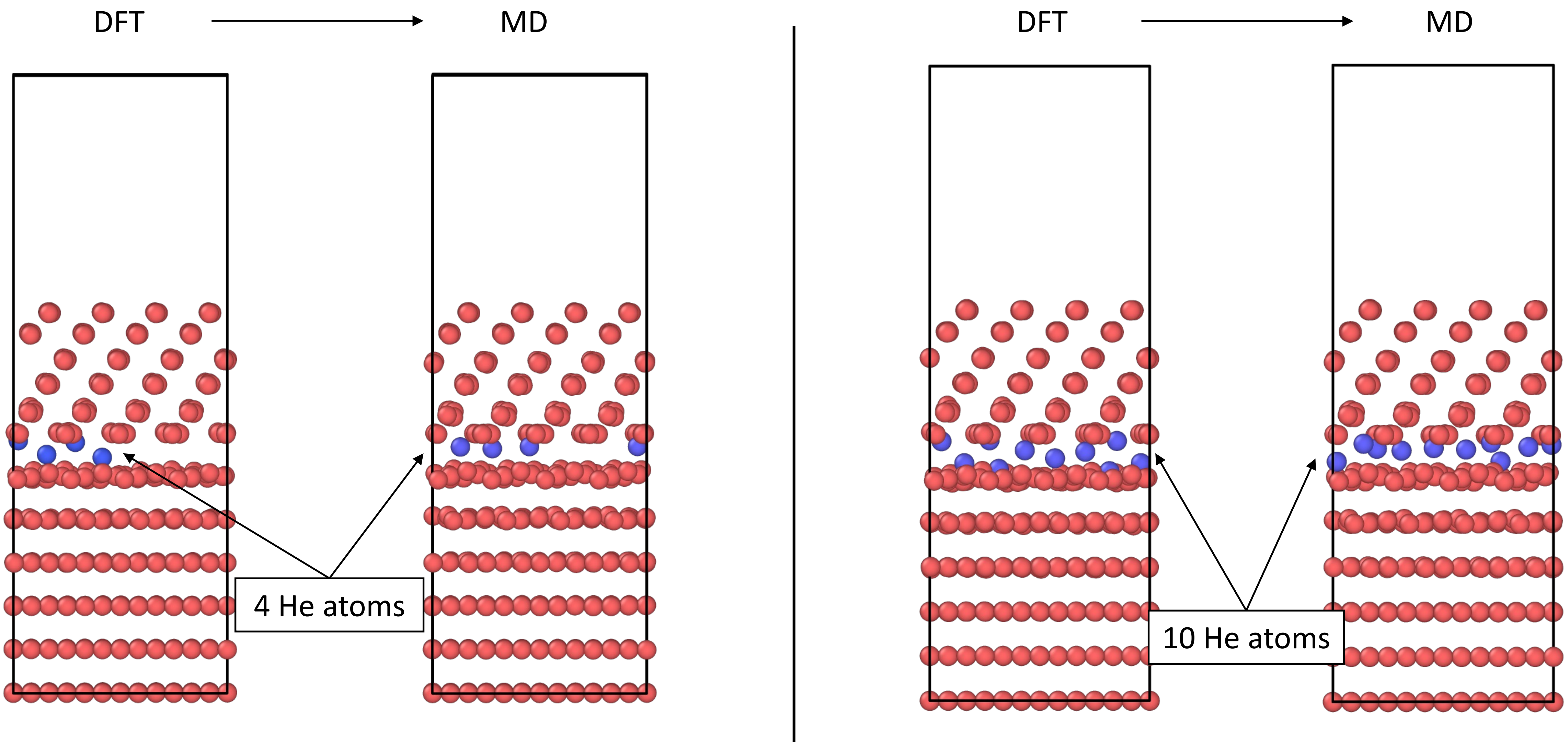
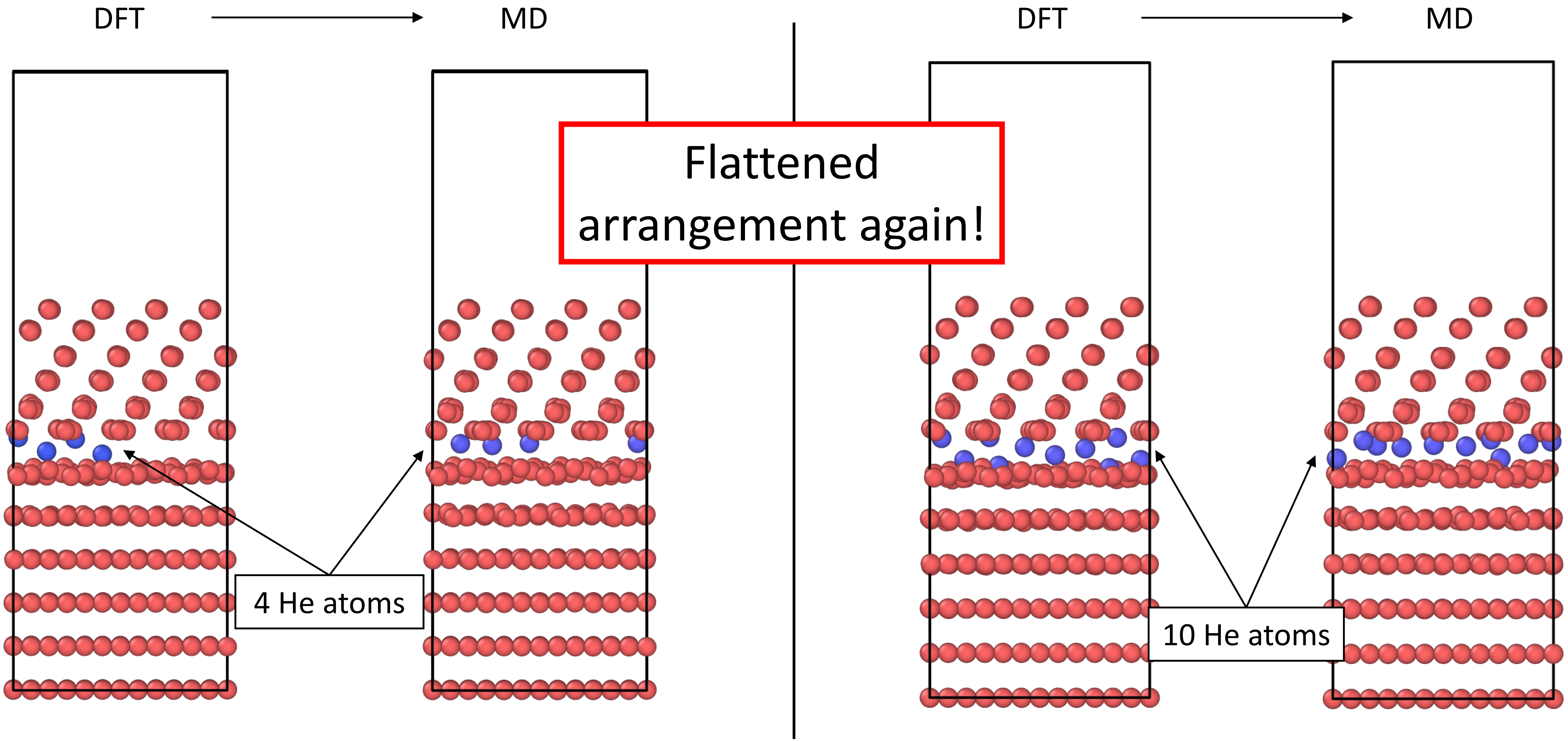

MD
Flattenned arrangement
Appreciable difference among He positions

Results



Results


DFT
MD
DFT
MD
Flattened arrangement again!
4 He atoms
10 He atoms

CONCLUSIONS

- Clearly motivated the study of self-healing in nanostructured W under the presence of He
- Great gain of computational time by means of a combined MD + DFT approach vs. DFT alone
- Energetic and structural analysis of the simultaneous presence of He, SIA and vacancy
- Study of defect migration barriers along the W(110) / W(112) interface to assess if it acts as an *effective diffusion channel* or it undergoes *GB decohesion*.
- Work in progress

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THANK YOU FOR YOUR ATTENTION!!!