



Propriedades Quânticas de Nanomateriais utilizando a Teoria do Funcional Densidade (DFT)

Pedro Venezuela
Marcio Costa



Outline



- Pseudopotentials : Where to get it? Which one to use?
- How to simulate a 2D material : Graphene
- Boron adatoms on Graphene
- Supercell

Pseudo Potentials



- <https://www.quantum-espresso.org/pseudopotentials>
- <http://theoossrv1.epfl.ch/Main/Pseudopotentials>
- <https://dalcorsogithub.io/pslibrary/>
- <https://www.materialscloud.org/discover/sssp/table/efficiency>

Pseudo Potentials



<https://www.materialscloud.org/discover/sssp/table/efficiency>

Standard solid-state pseudopotentials (SSSP)

SSSP Efficiency (version 1.1)

$$\Delta_{\text{eff}} = 0.44 \text{ meV}$$

[Download Cutoffs table](#)

 Pseudos

Switch to SSSP Precision

Updates v1.1 beta



Pseudo Potentials



Cohesion Energy (E_{coh})

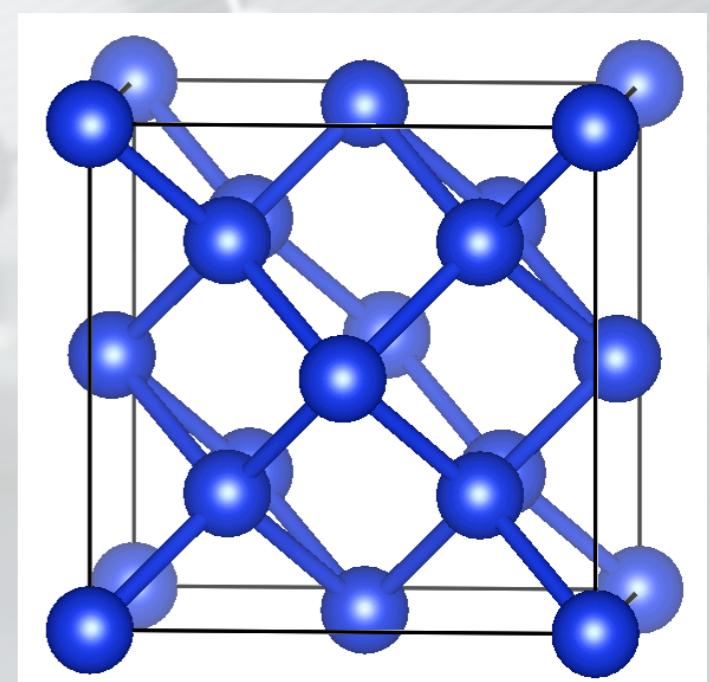
$$E_{coh} = \frac{E_{tot} - \sum_N E_{iso}}{N}$$



Cohesion Energy (E_{coh})

$$E_{coh} = \frac{E_{tot} - \sum_N E_{iso}}{N}$$

E_{tot} total energy of the periodic calculation





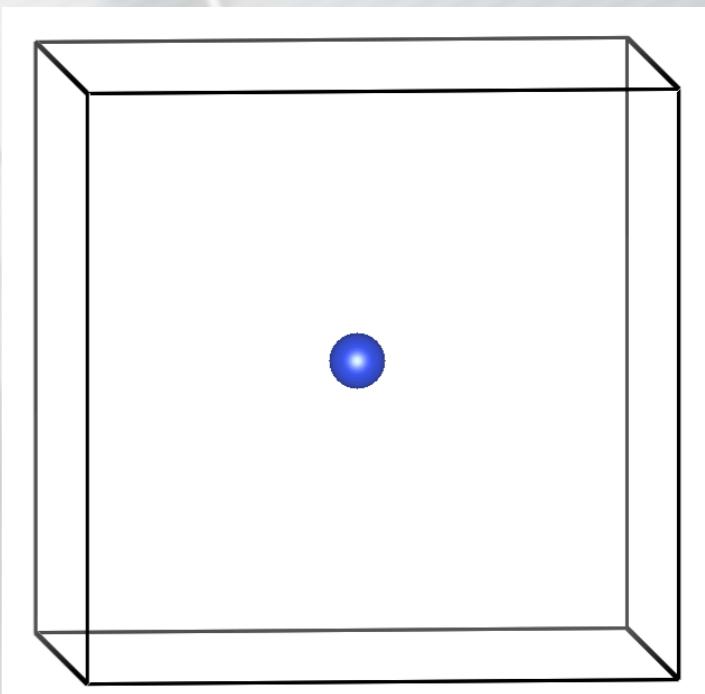
Pseudo Potentials

Cohesion Energy (E_{coh})

$$E_{coh} = \frac{E_{tot} - \sum_N E_{iso}}{N}$$

E_{tot} total energy of the periodic calculation

E_{iso} total energy of an isolated calculation





Pseudo Potentials

Cohesion Energy (E_{coh})

$$E_{coh} = \frac{E_{tot} - \sum_N E_{iso}}{N}$$

E_{tot} total energy of the periodic calculation

E_{iso} total energy of an isolated calculation

N total number of atoms in the periodic system



Pseudo Potentials

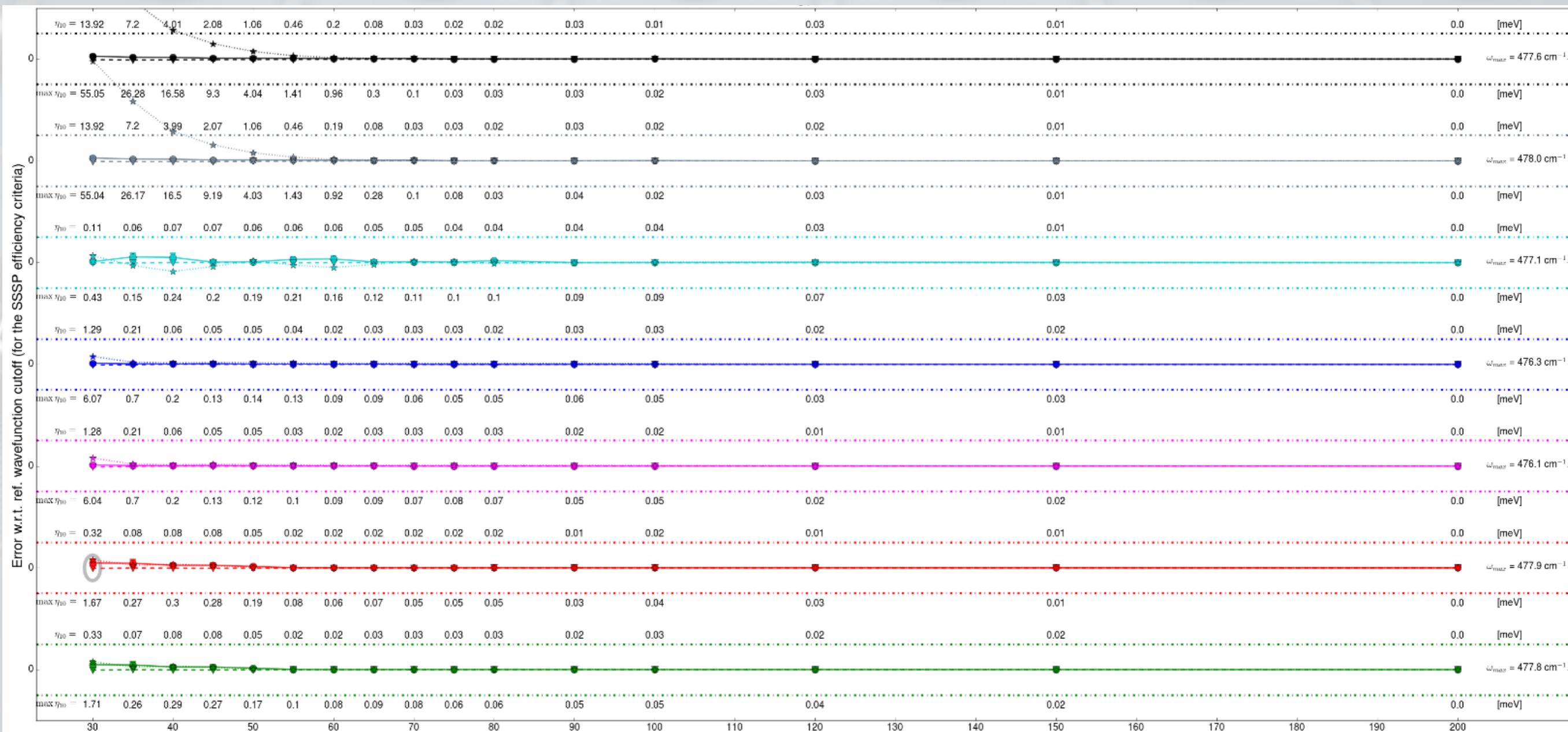
SSSP Criteria

	SSSP Efficiency	SSSP Precision	notes
Phonon frequencies ($\delta\bar{\omega}$)	< 2%	< 1%	(% → cm^{-1} if $\omega_{\max} < 100 \text{ cm}^{-1}$)
Cohesive energy (δE_{coh})	< 2 meV/atom	< 2 meV/atom	
Pressure (δV_{press})	< 1%	< 0.5%	in terms of volume differences
Band structure (η_{10})	< 10 meV	< 10 meV	
Band structure (max η_{10})	< 20 meV	< 20 meV	
Equation of state (Δ -factor)	< 1 meV/atom (if possible)	smallest	



Pseudo Potentials

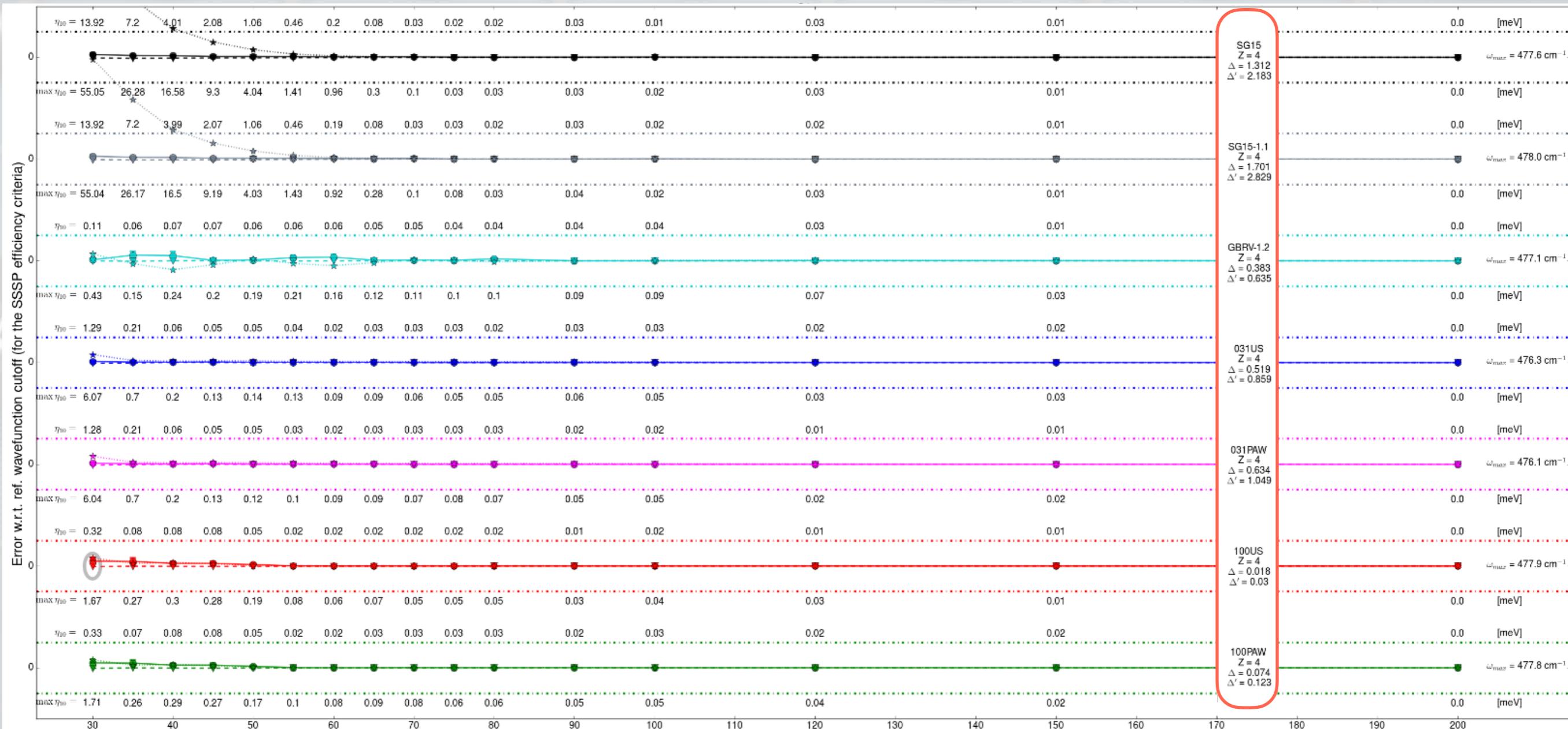
Silicon





Pseudo Potentials

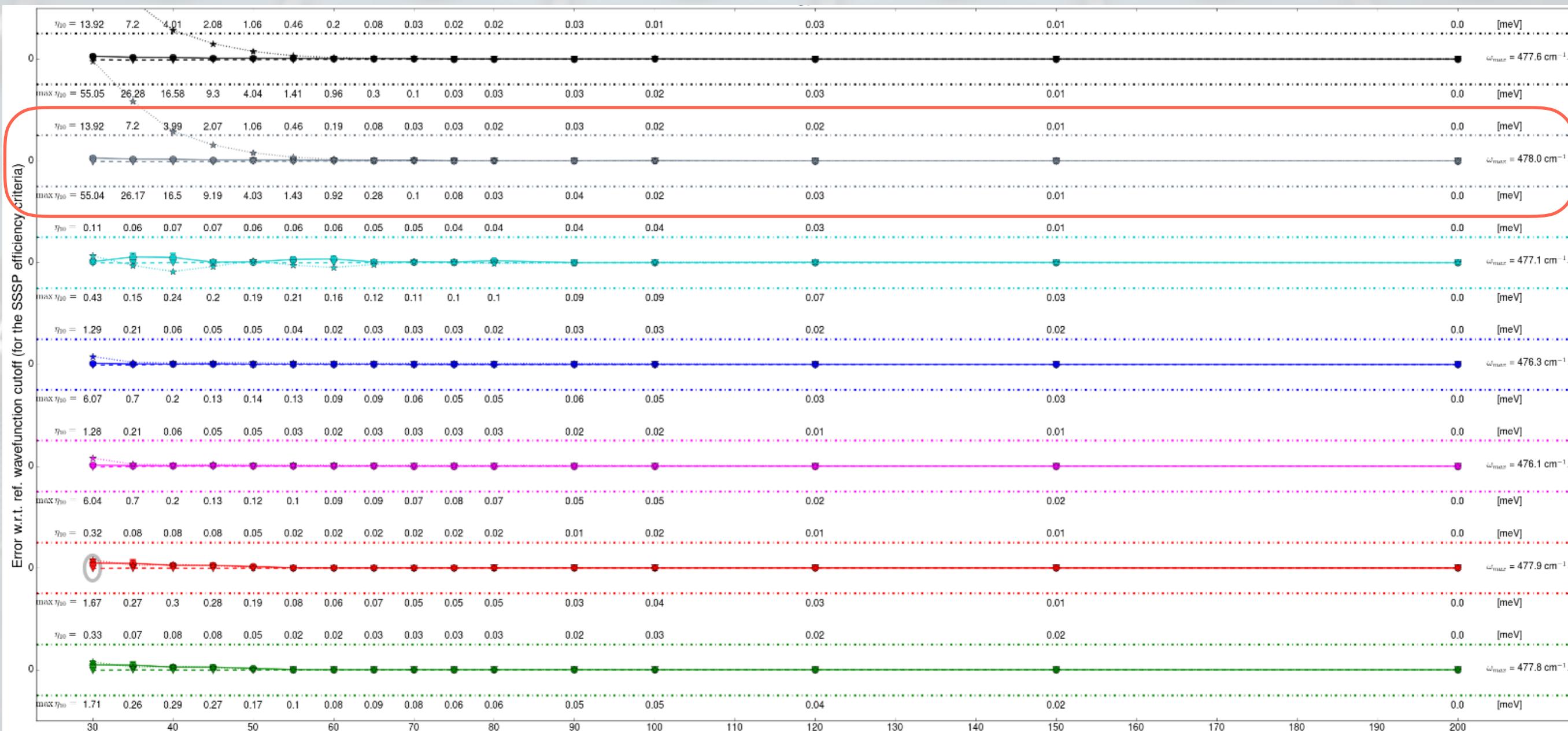
Silicon





Pseudo Potentials

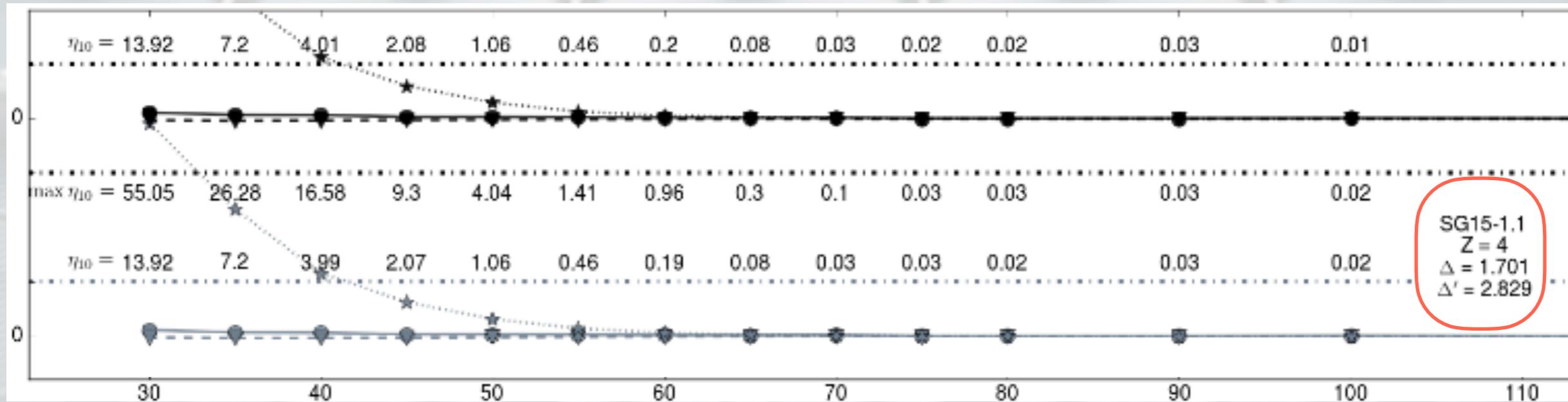
Silicon



Pseudo Potentials



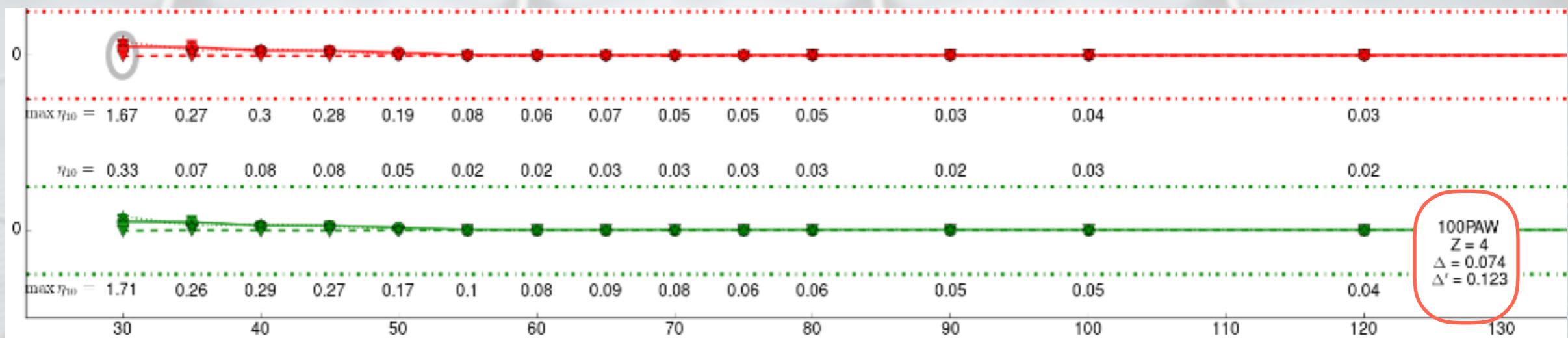
Silicon





Pseudo Potentials

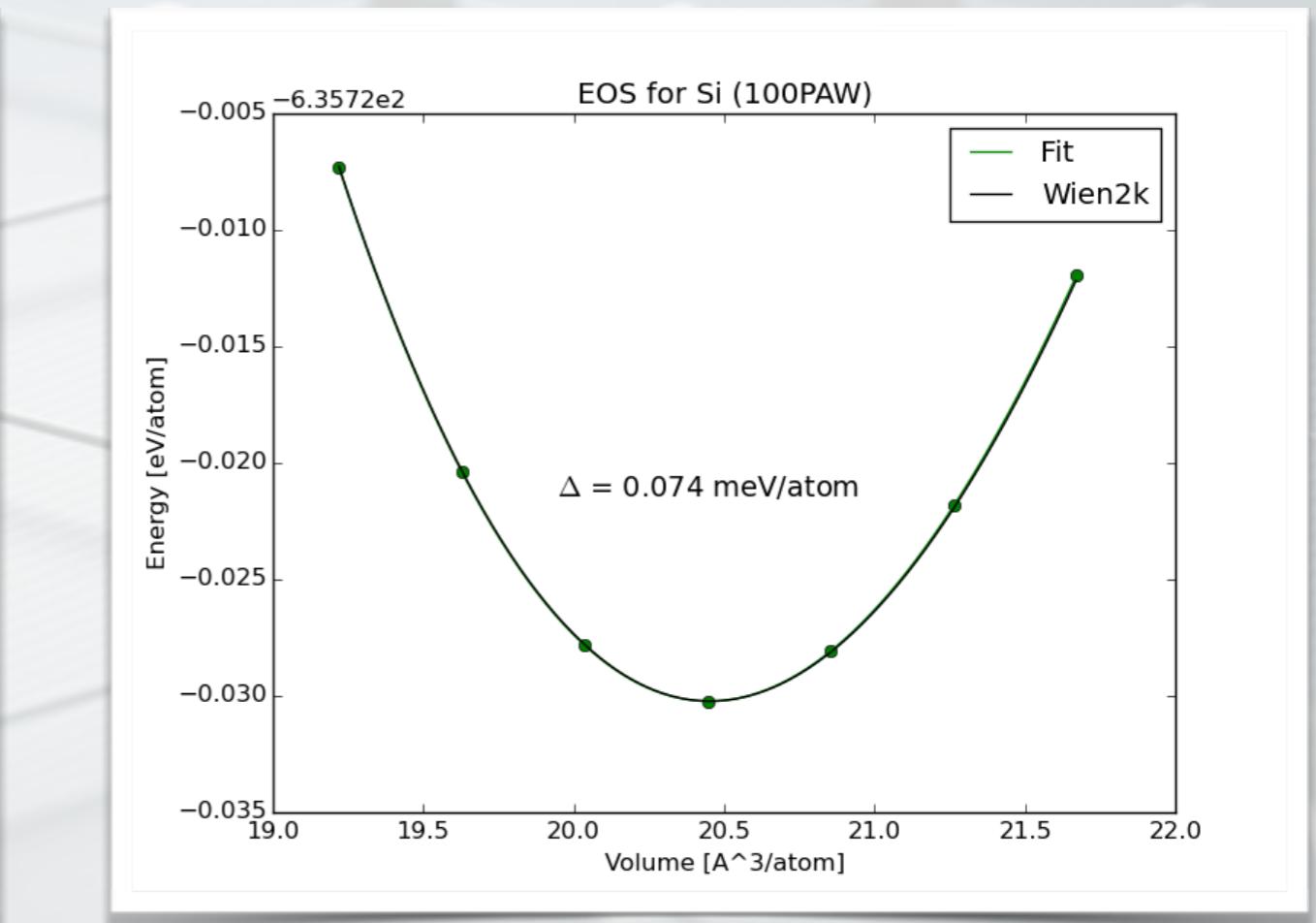
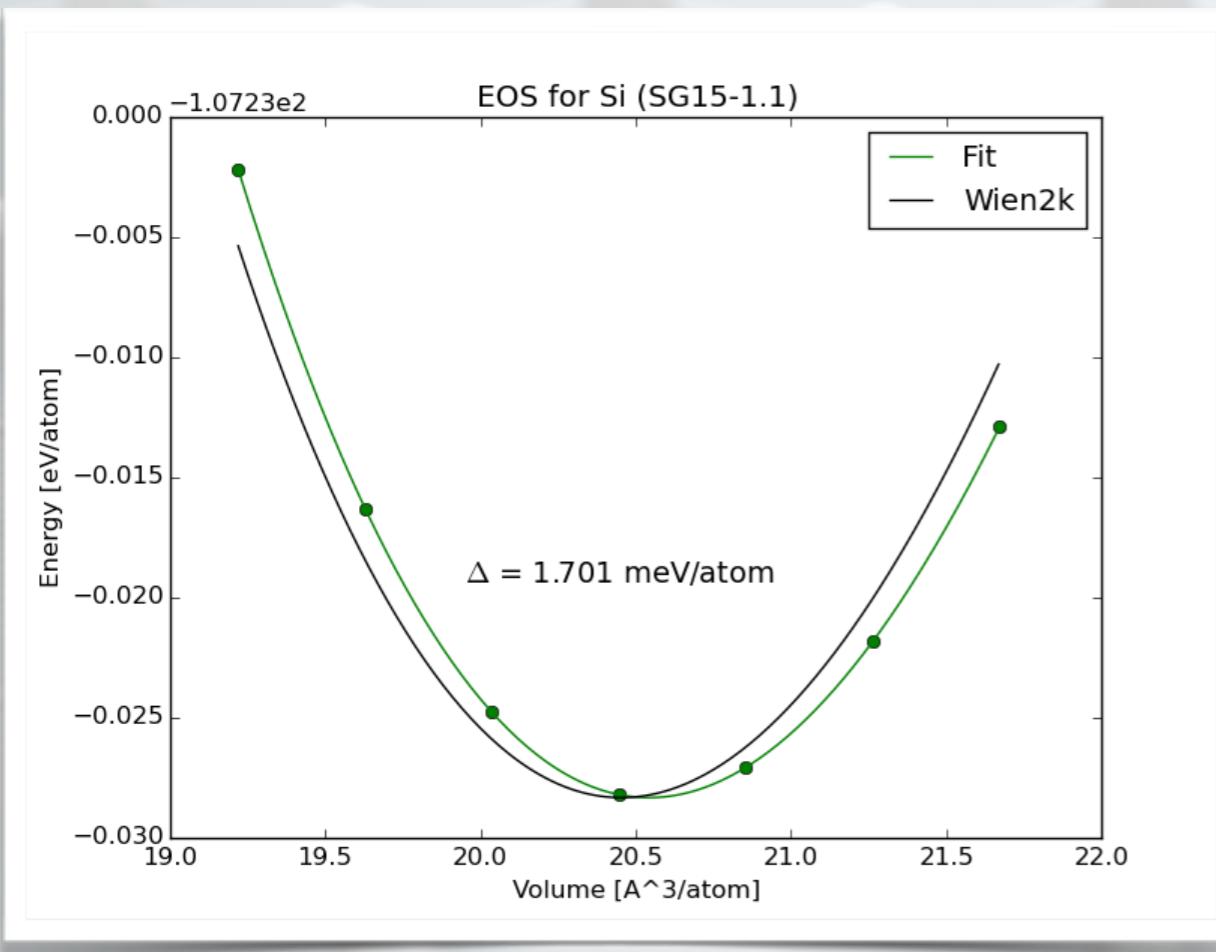
Silicon



Pseudo Potentials



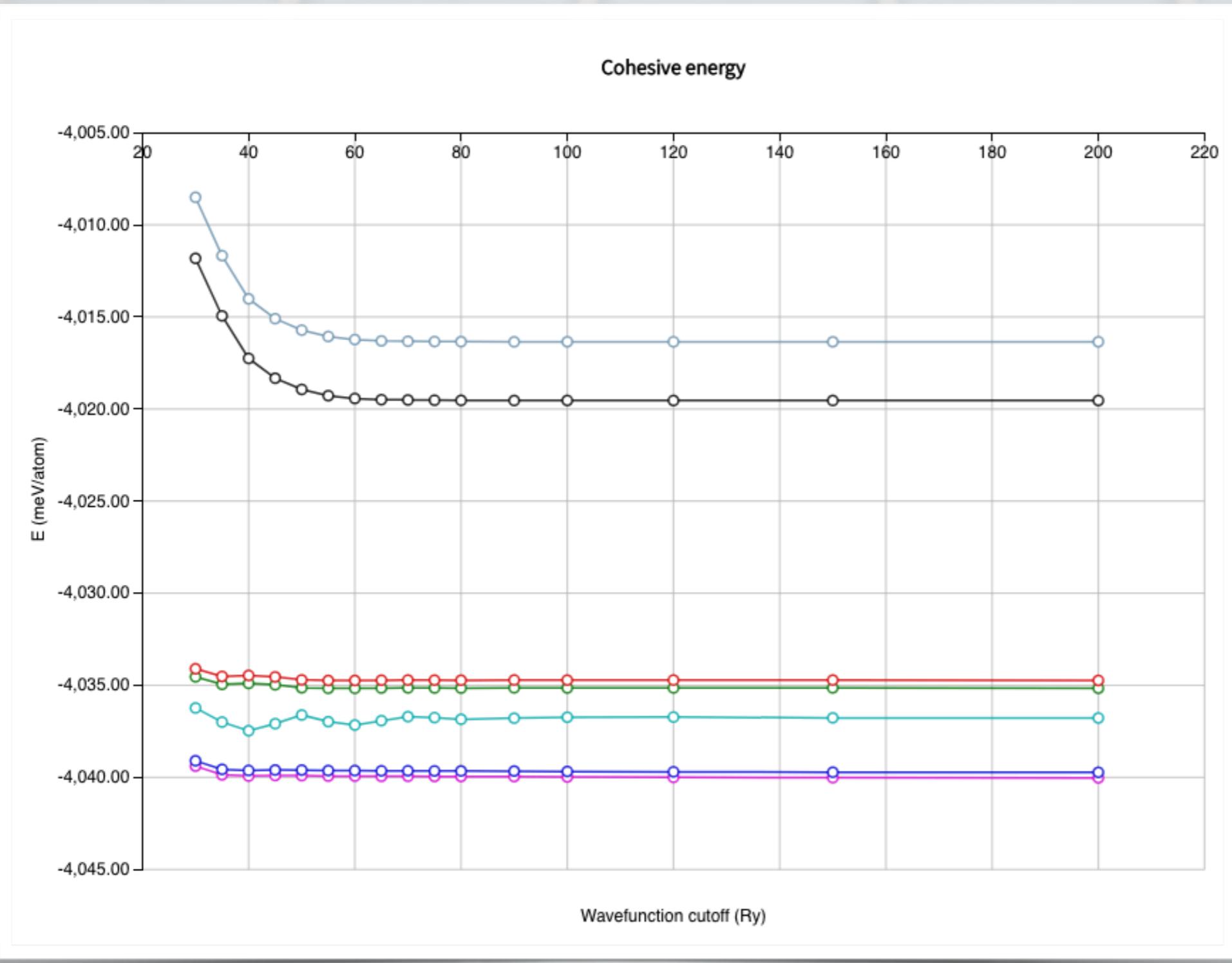
Silicon





Pseudo Potentials

Silicon

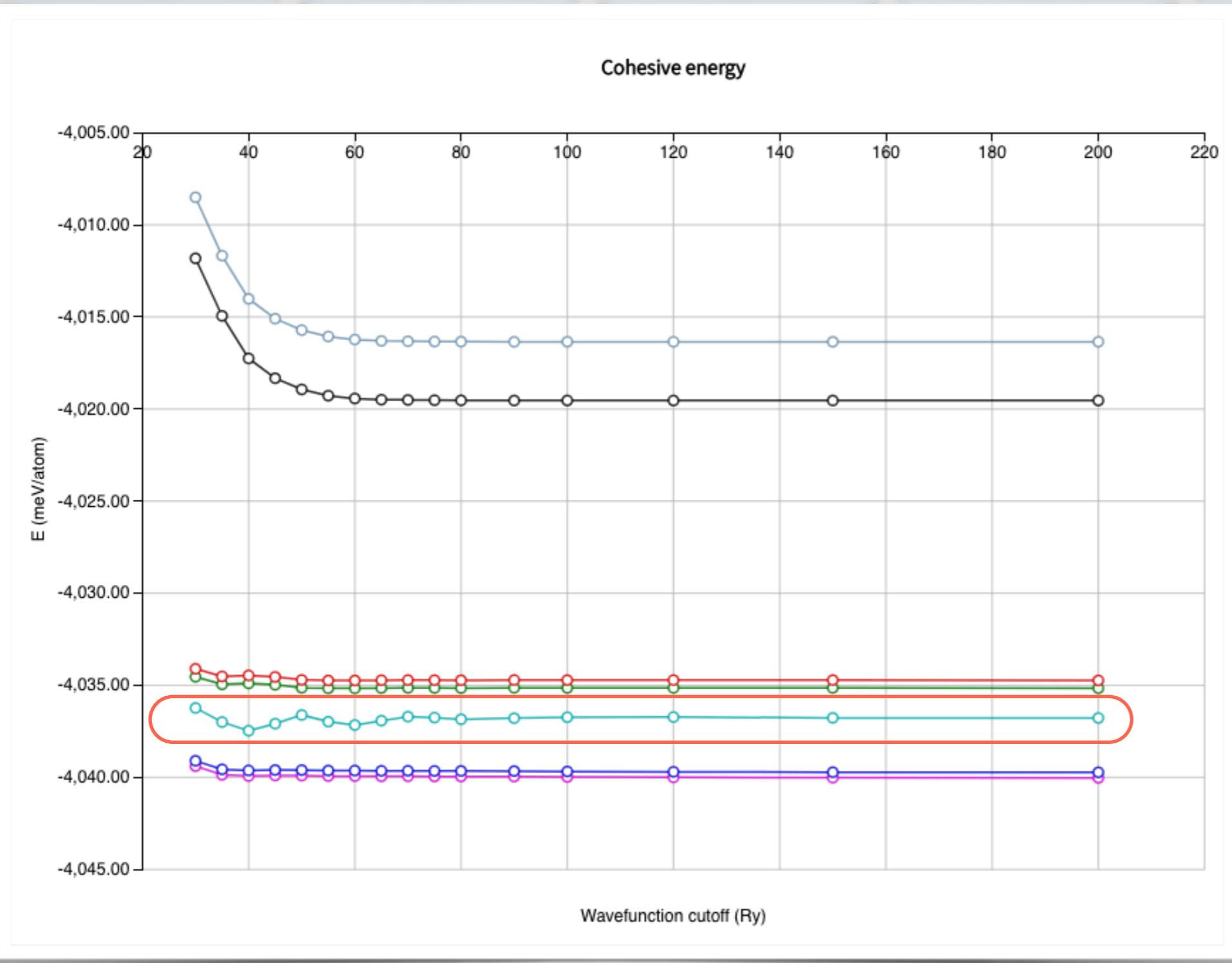


- GBRV-1.2 (US), dual=8
- SG15 (NC), dual=4
- SG15-1.1 (NC), dual=4
- pslibrary.0.3.1 PAW (high acc.), dual=8
- pslibrary.0.3.1 US (high acc.), dual=8
- pslibrary.1.0.0 PAW (high acc.), dual=8
- pslibrary.1.0.0 US (high acc.), dual=8



Pseudo Potentials

Silicon

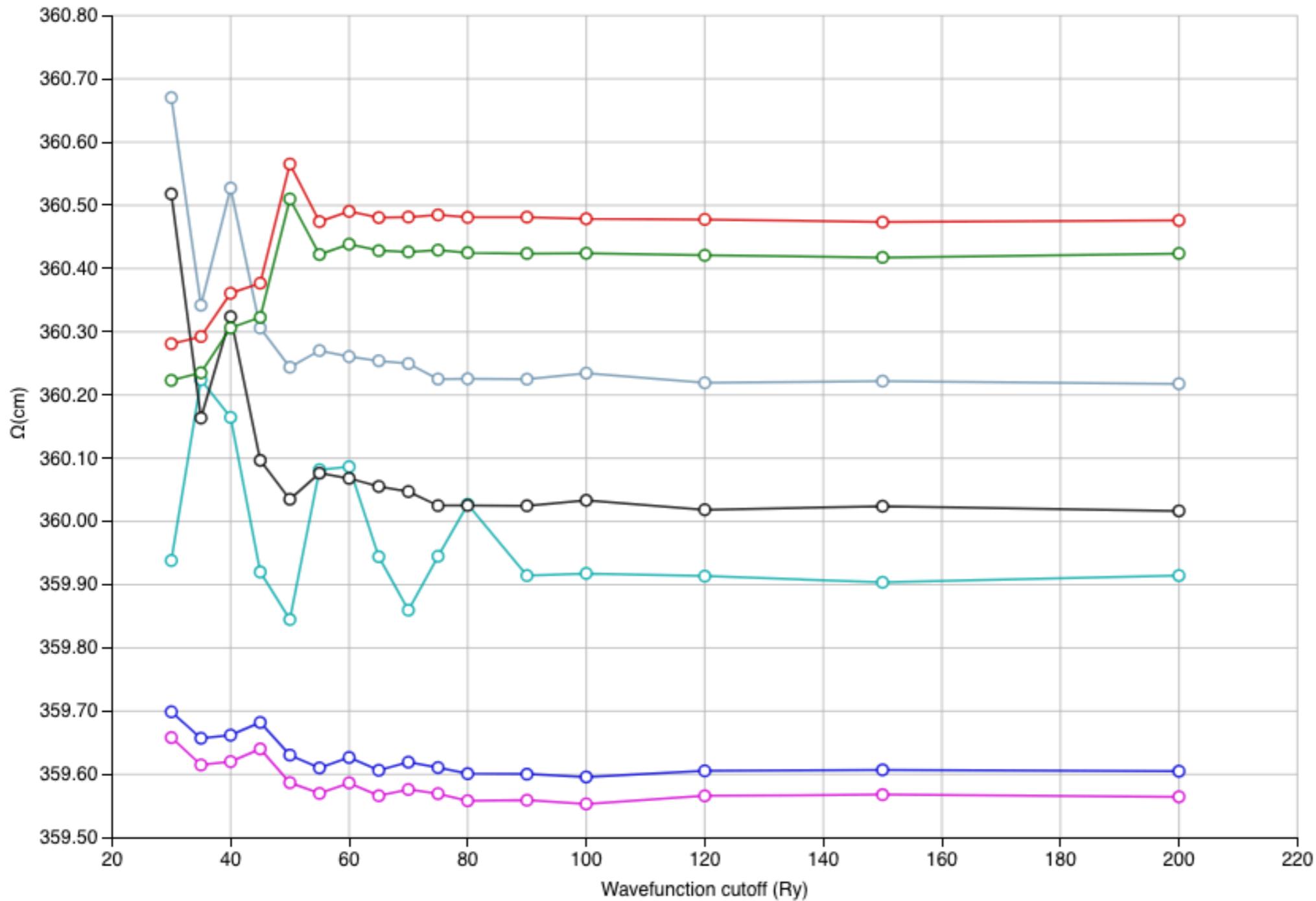




Pseudo Potentials

Silicon

Phonons



Legend:

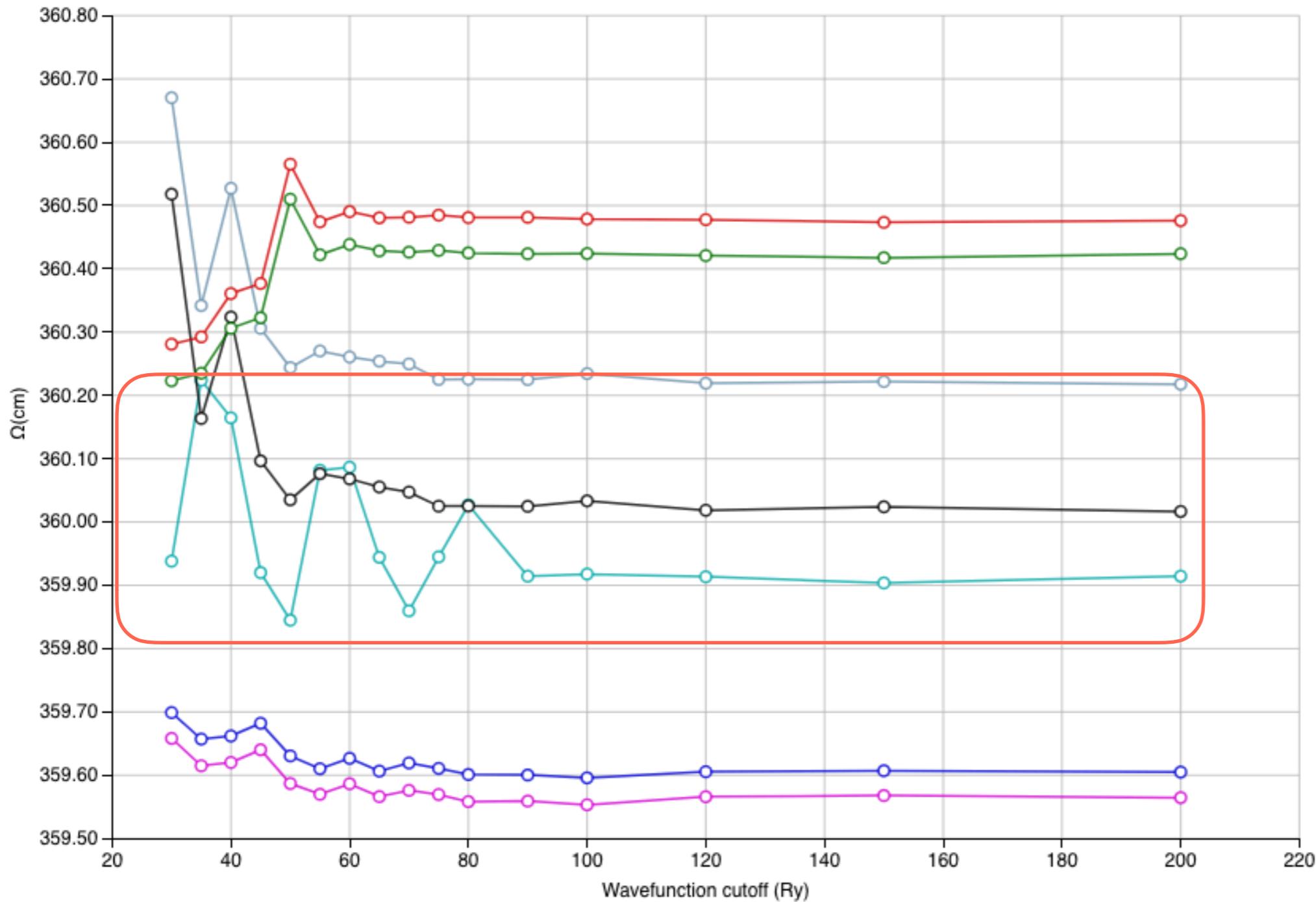
- GBRV-1.2 (US), dual=8
- SG15 (NC), dual=4
- SG15-1.1 (NC), dual=4
- pslibrary.0.3.1 PAW (high acc.), dual=8
- pslibrary.0.3.1 US (high acc.), dual=8
- pslibrary.1.0.0 PAW (high acc.), dual=8
- pslibrary.1.0.0 US (high acc.), dual=8



Pseudo Potentials

Silicon

Phonons

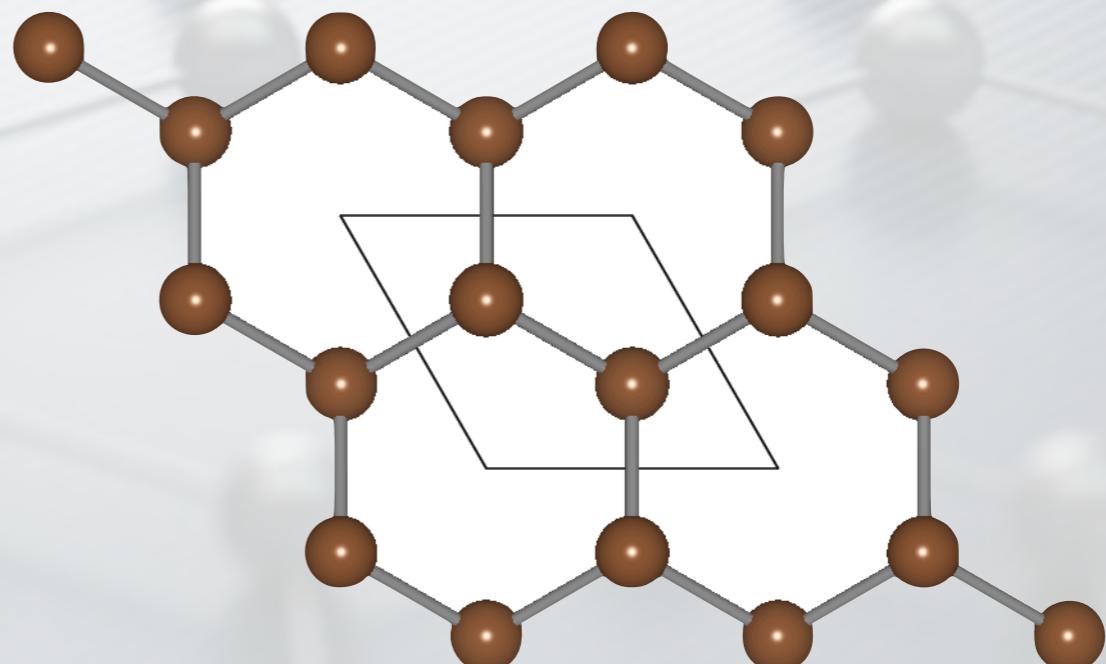


- GBRV-1.2 (US), dual=8
- SG15 (NC), dual=4
- SG15-1.1 (NC), dual=4
- pslibrary.0.3.1 PAW (high acc.), dual=8
- pslibrary.0.3.1 US (high acc.), dual=8
- pslibrary.1.0.0 PAW (high acc.), dual=8
- pslibrary.1.0.0 US (high acc.), dual=8



Graphene

- Band Structure
- Total and projected density of states
- Carbon phase diagram: Diamond X Honeycomb
- Phonons

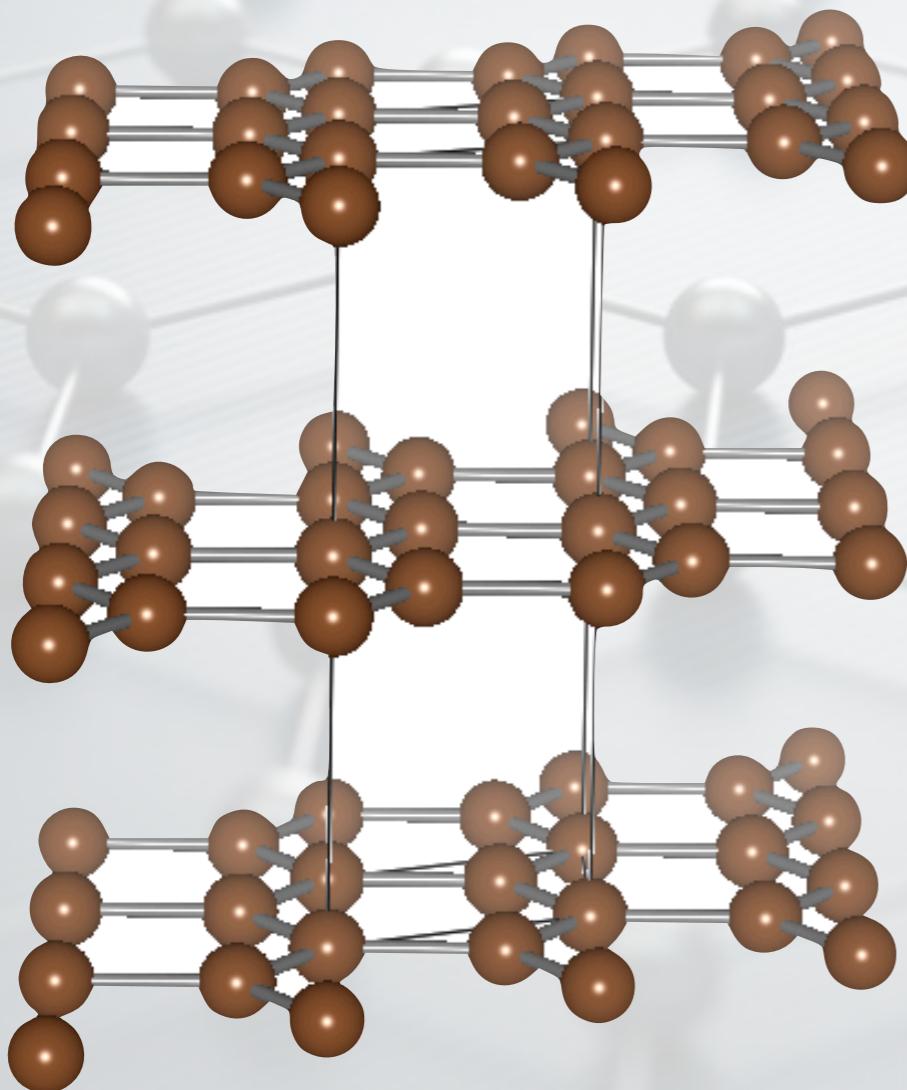




Graphene

How to simulate a 2D material?

Graphite

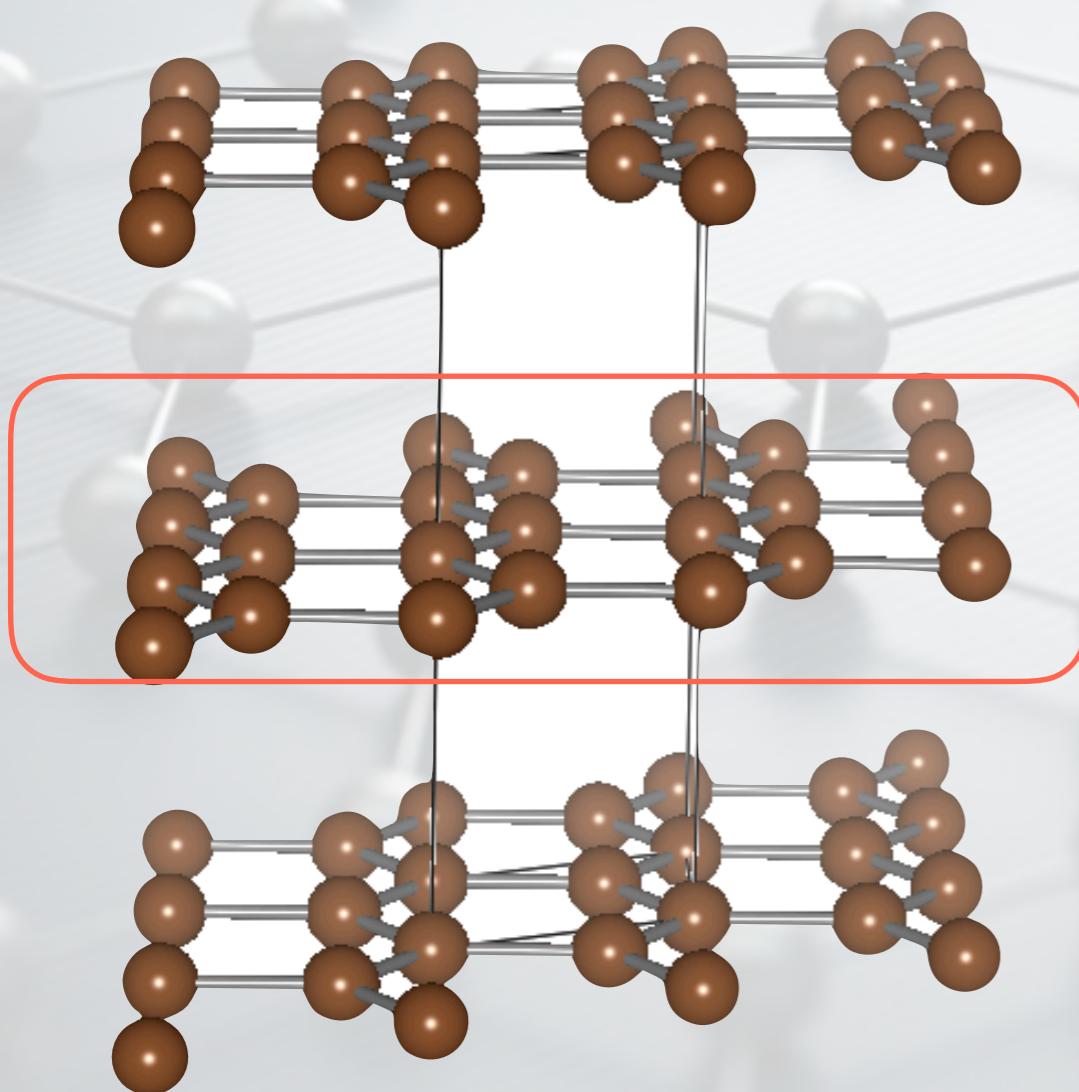




Graphene

How to simulate a 2D material?

Graphite

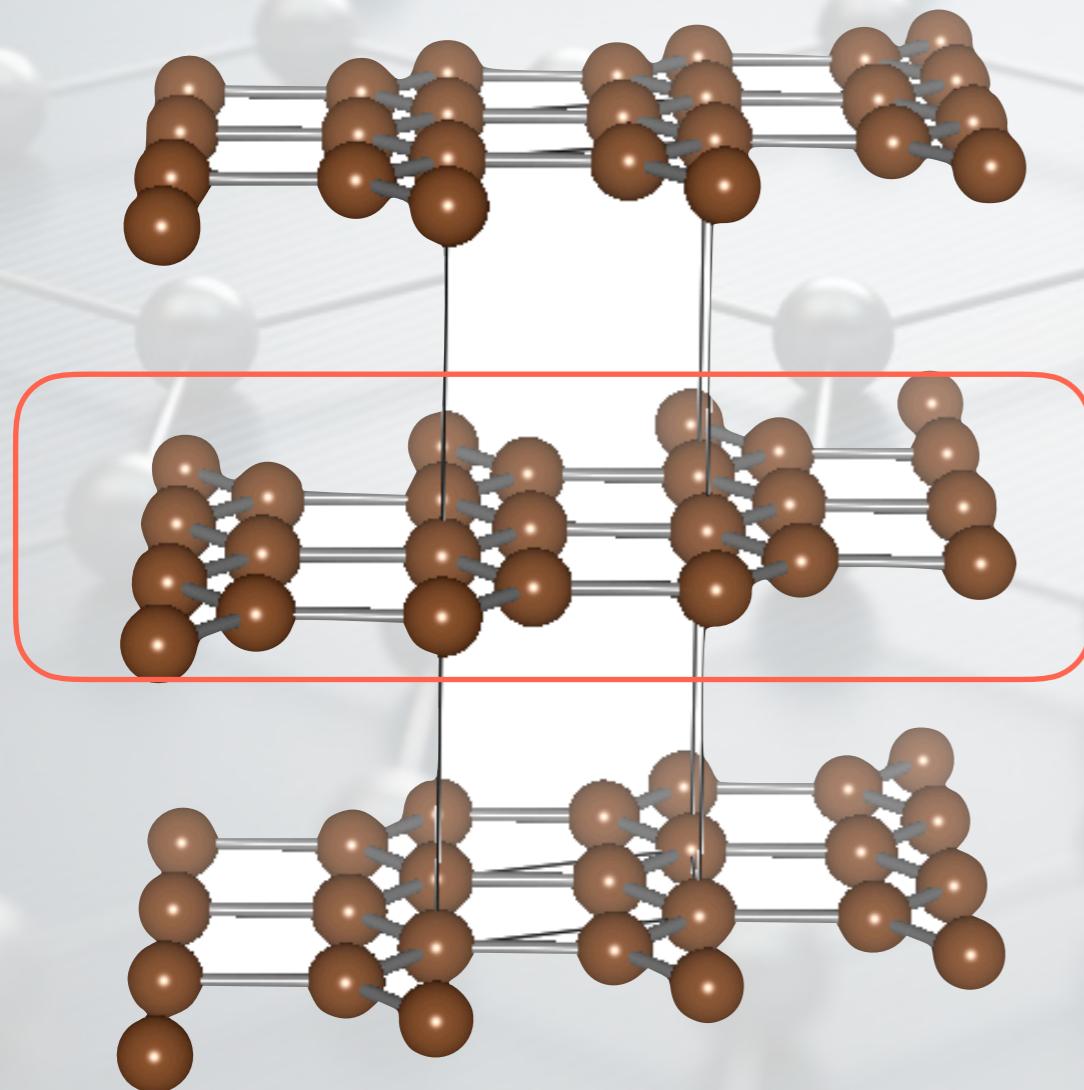


Graphene

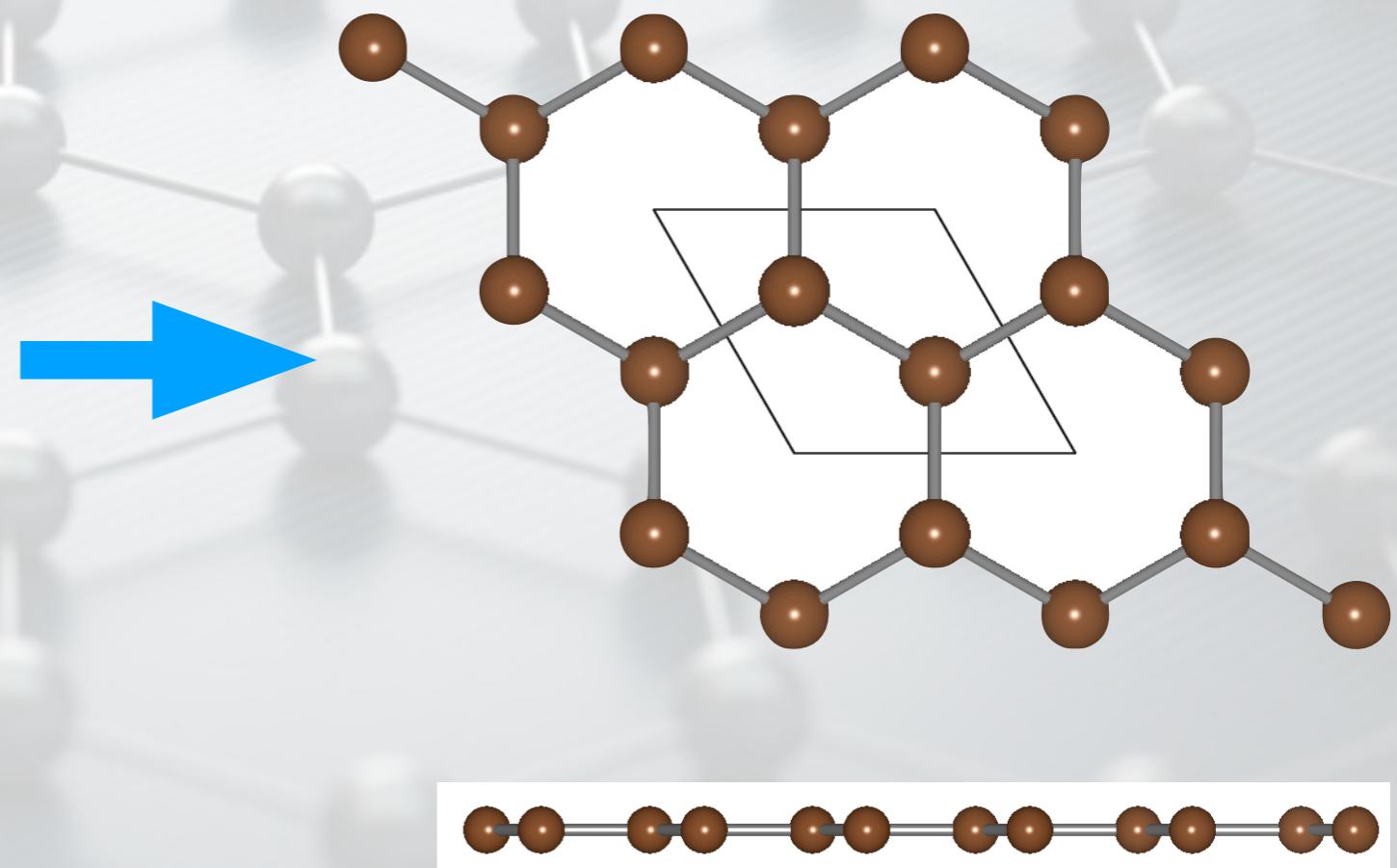


How to simulate a 2D material?

Graphite



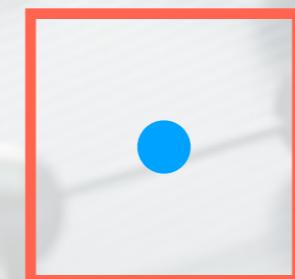
Gaphene





How to simulate a 2D material?

Periodic Boundary Conditions

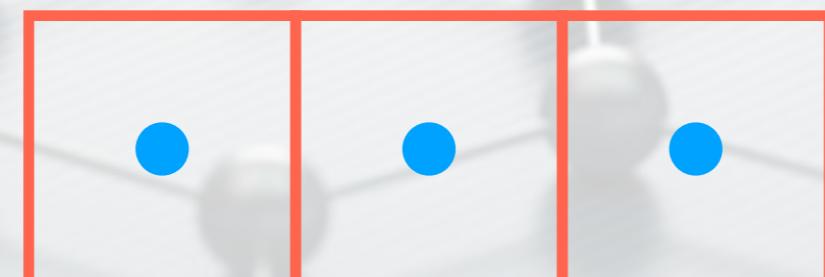


Graphene



How to simulate a 2D material?

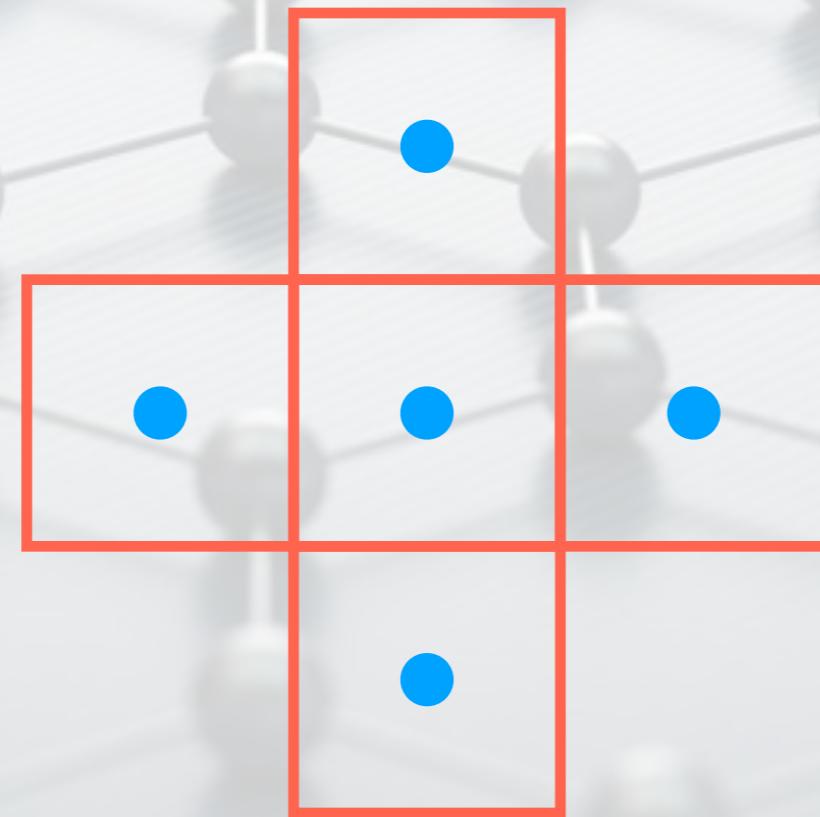
Periodic Boundary Conditions





How to simulate a 2D material?

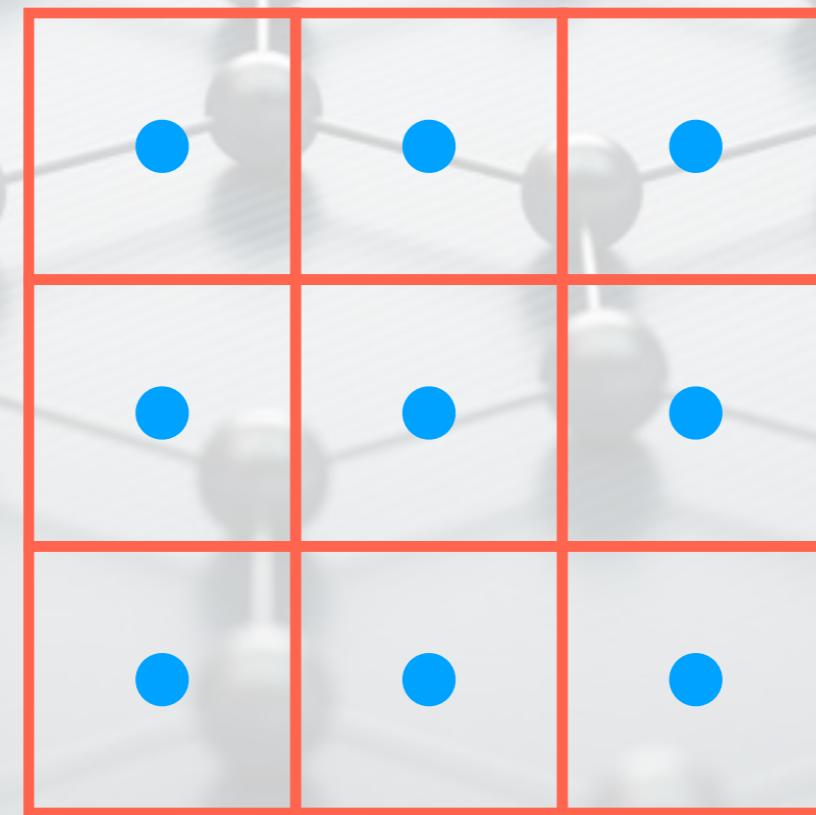
Periodic Boundary Conditions





How to simulate a 2D material?

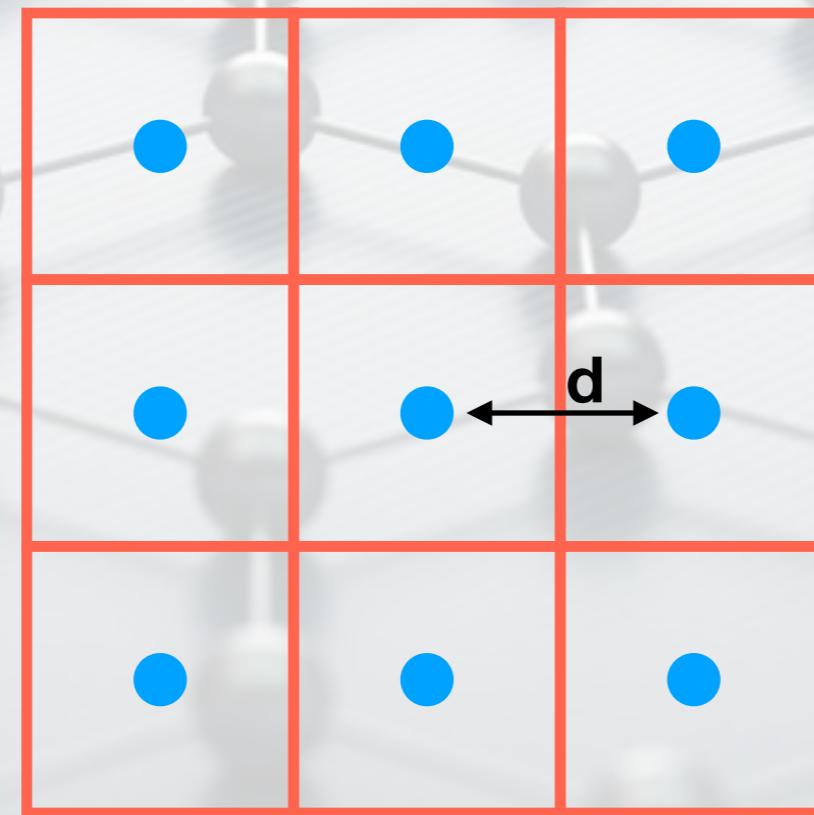
Periodic Boundary Conditions





How to simulate a 2D material?

Periodic Boundary Conditions

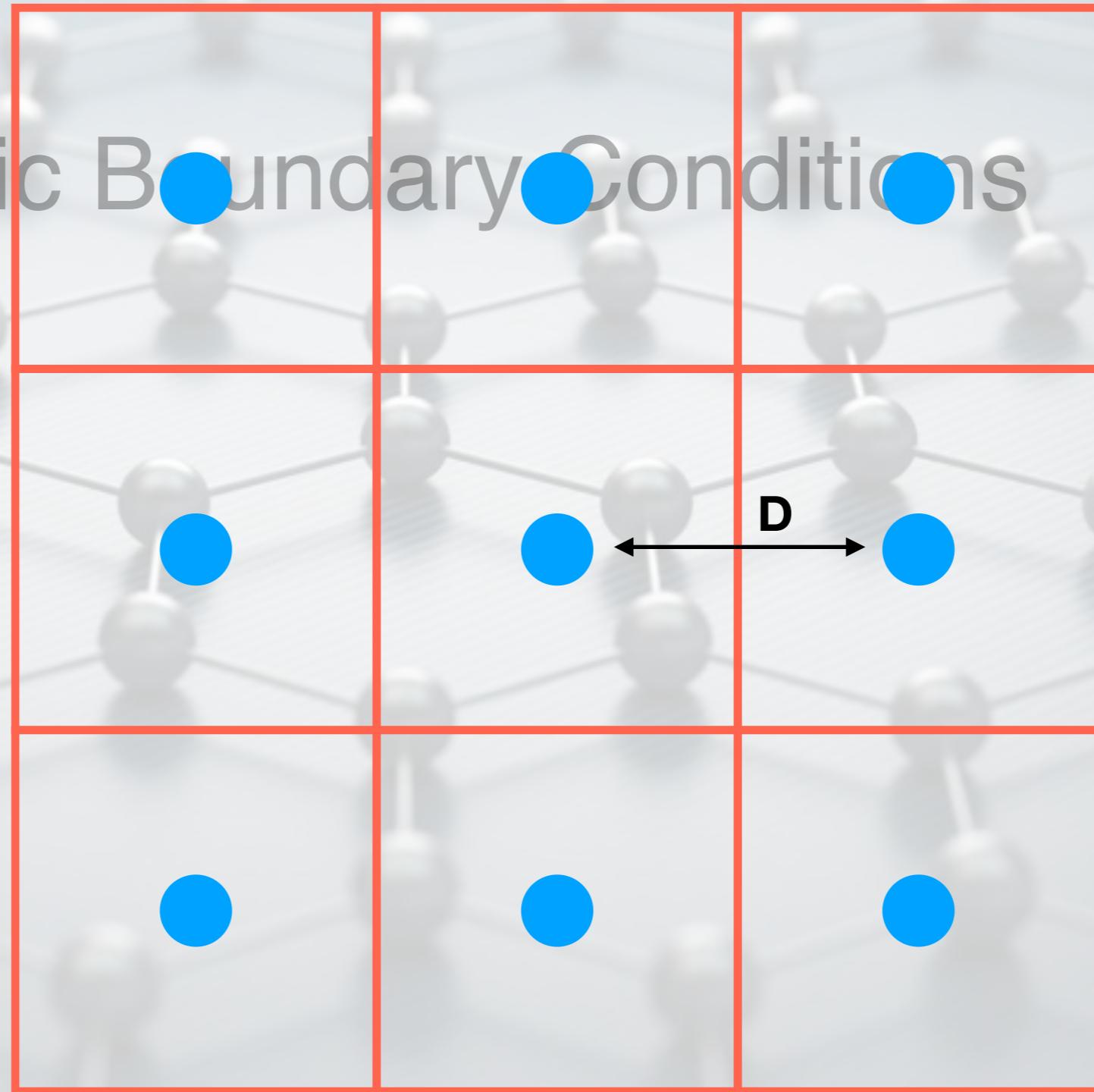


Graphene



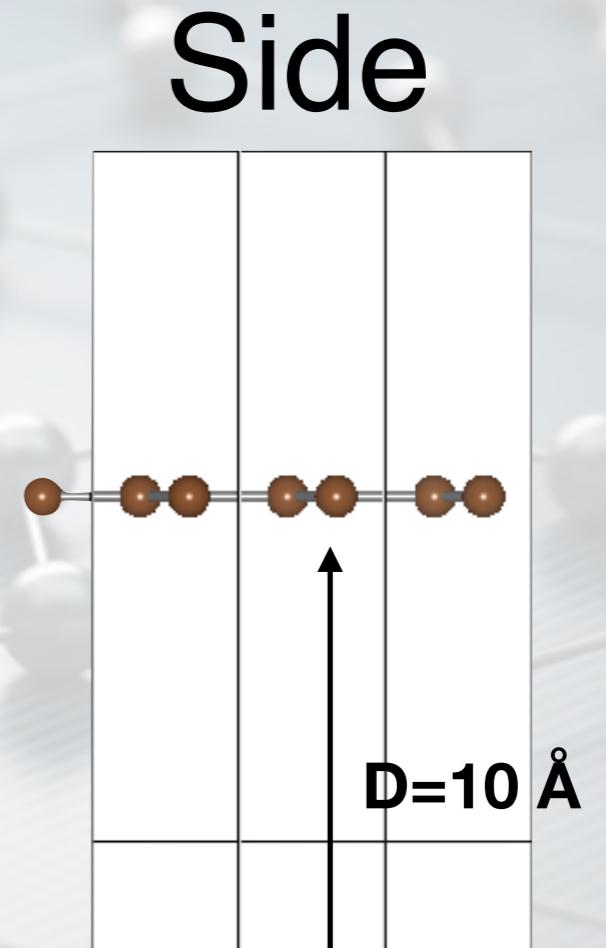
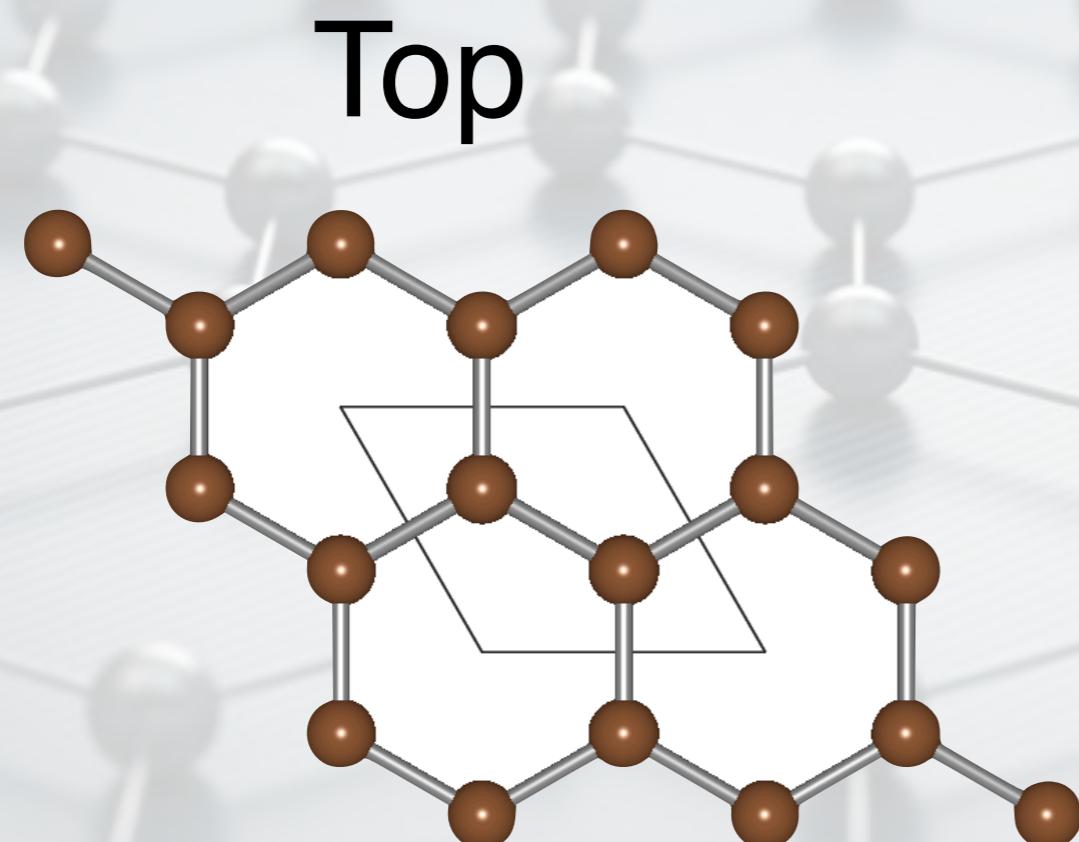
How to simulate a 2D material?

Periodic Boundary Conditions



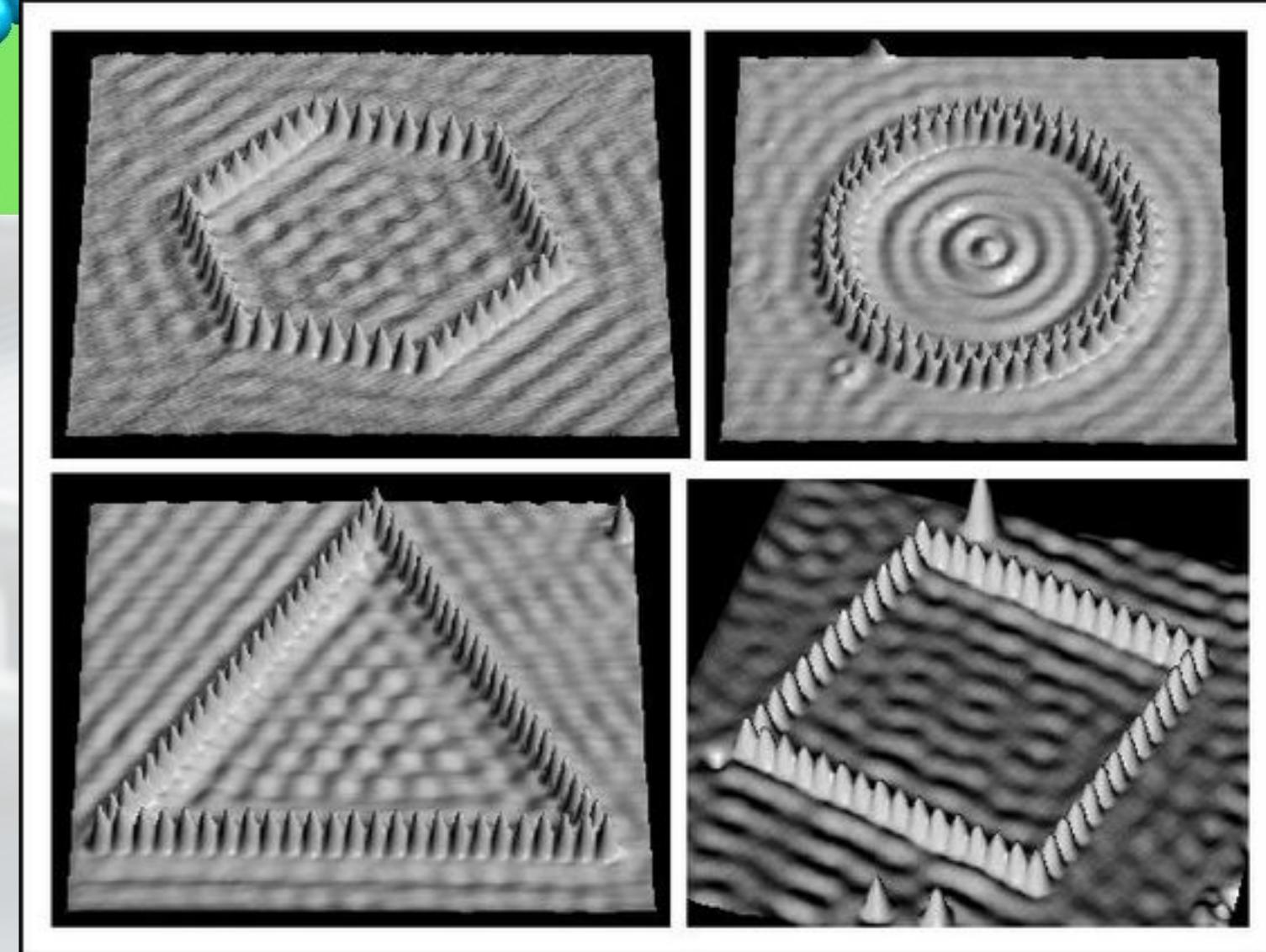
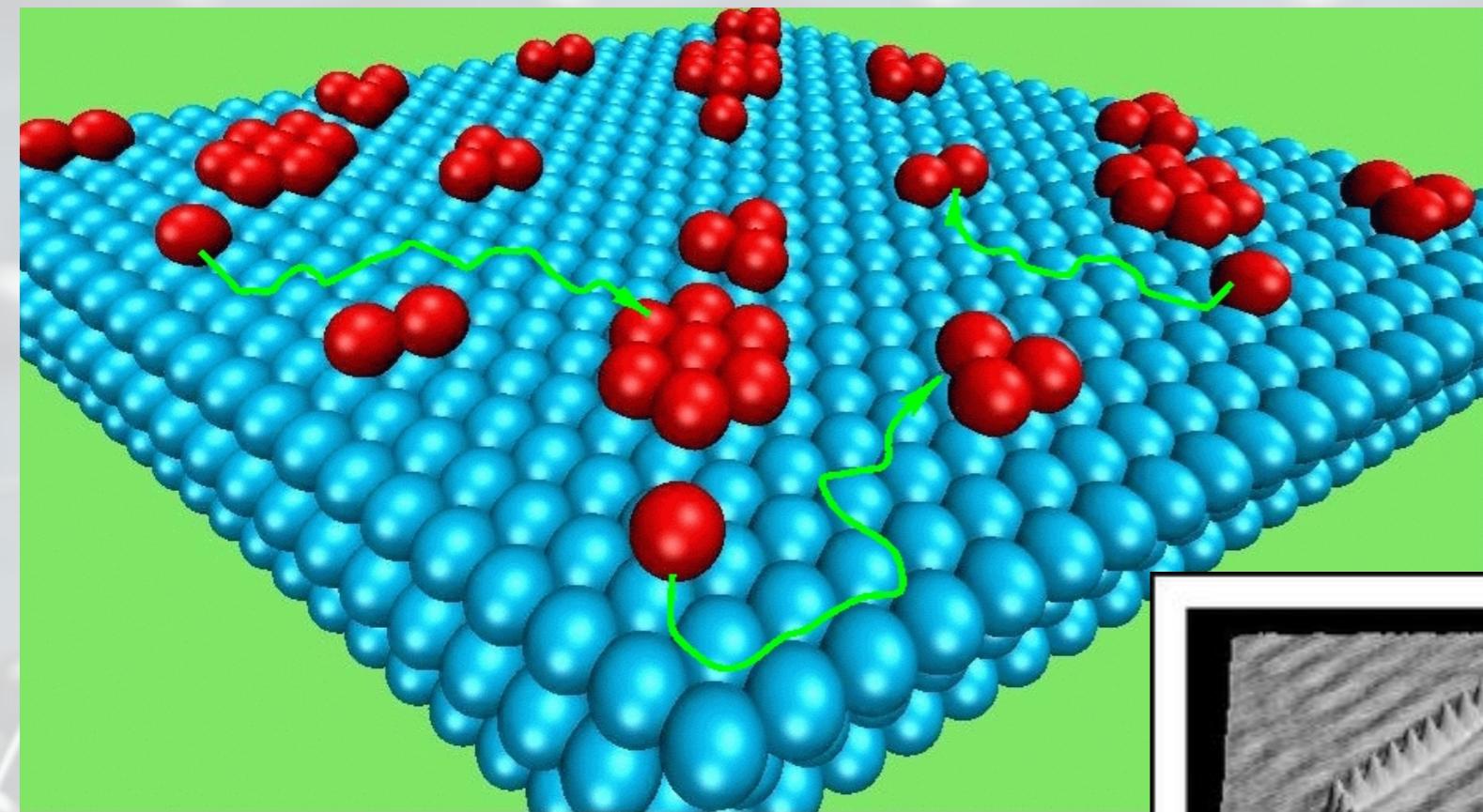


How to simulate a 2D material?

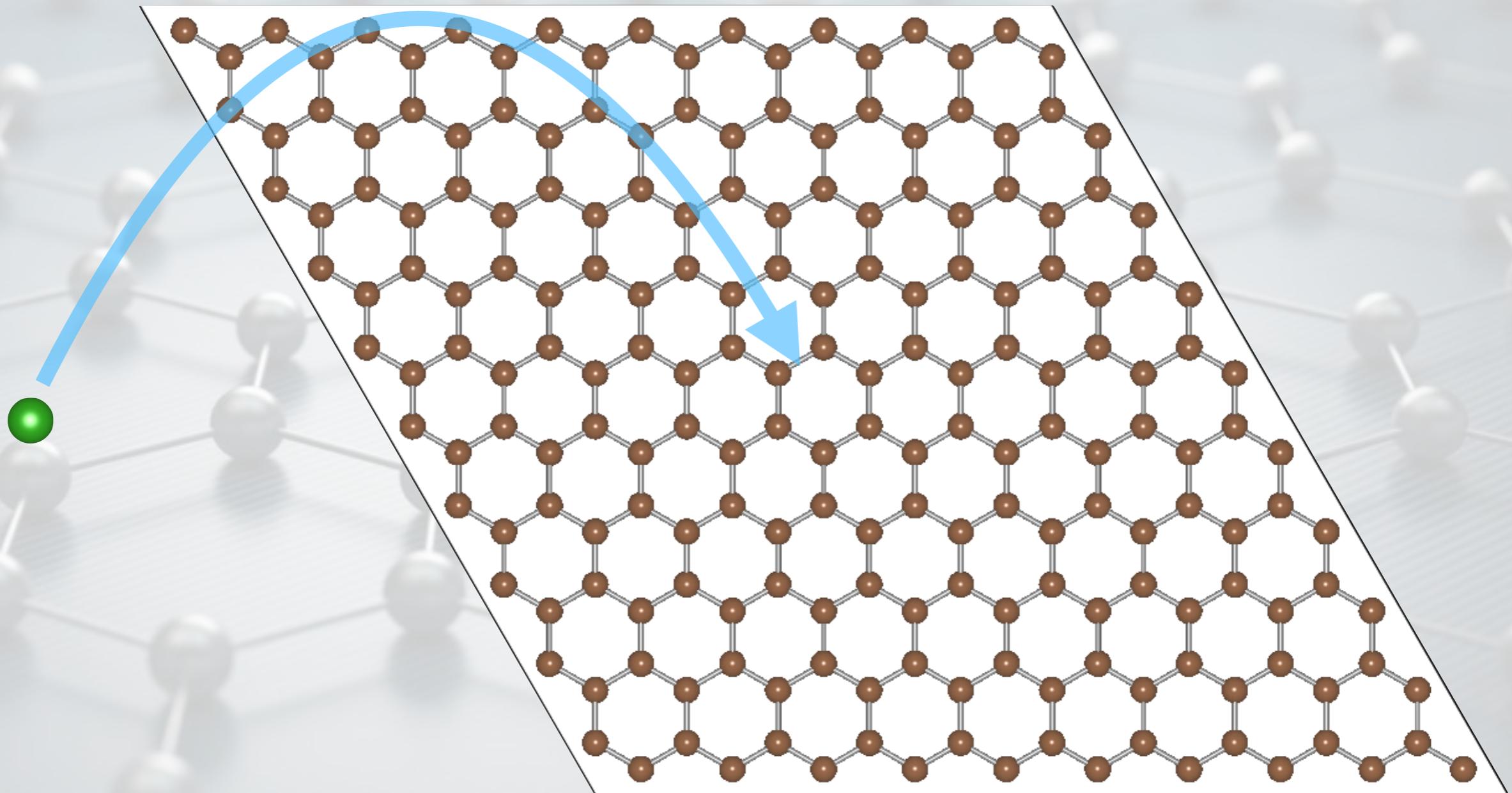




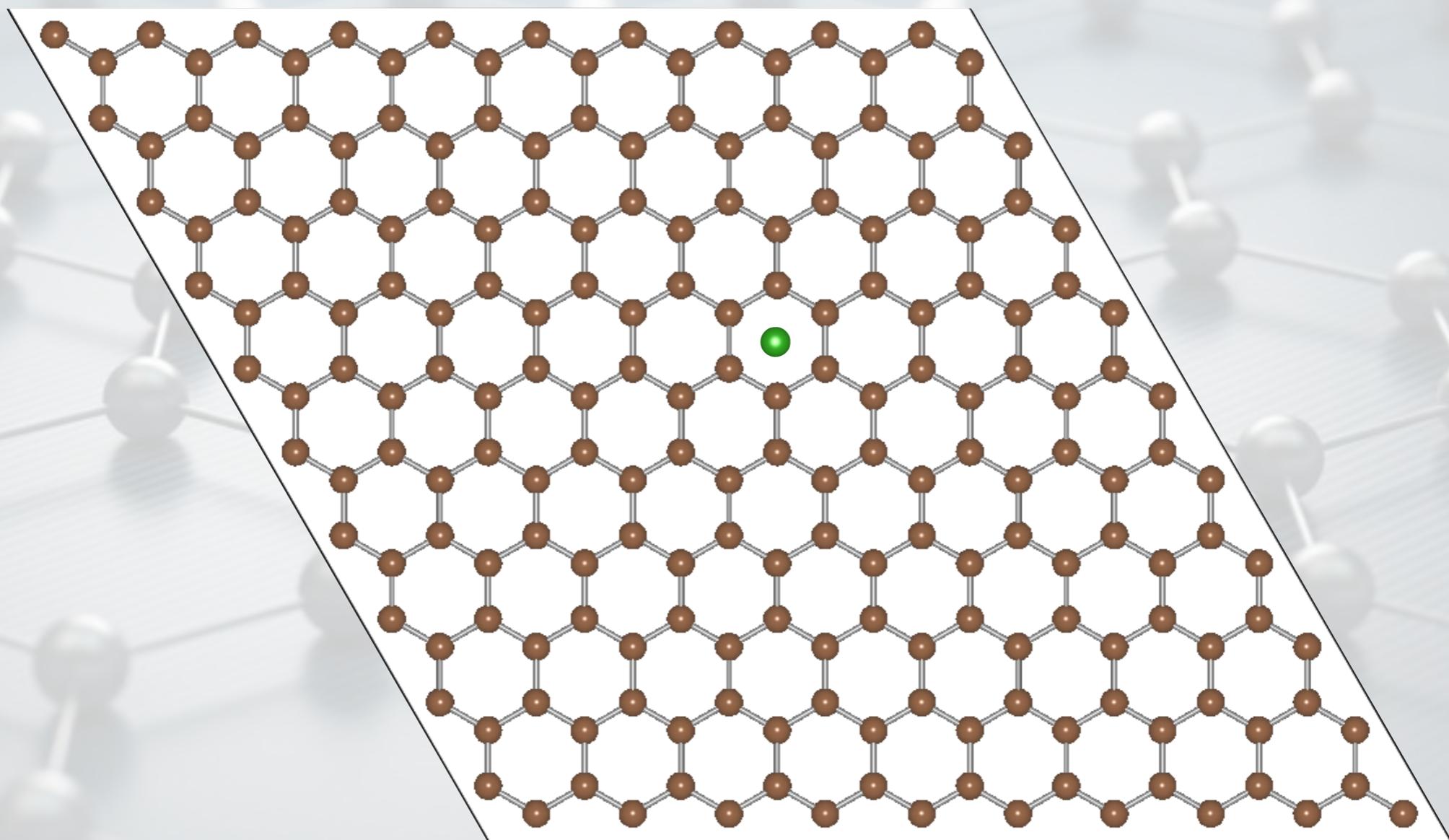
Boron adatoms on graphene



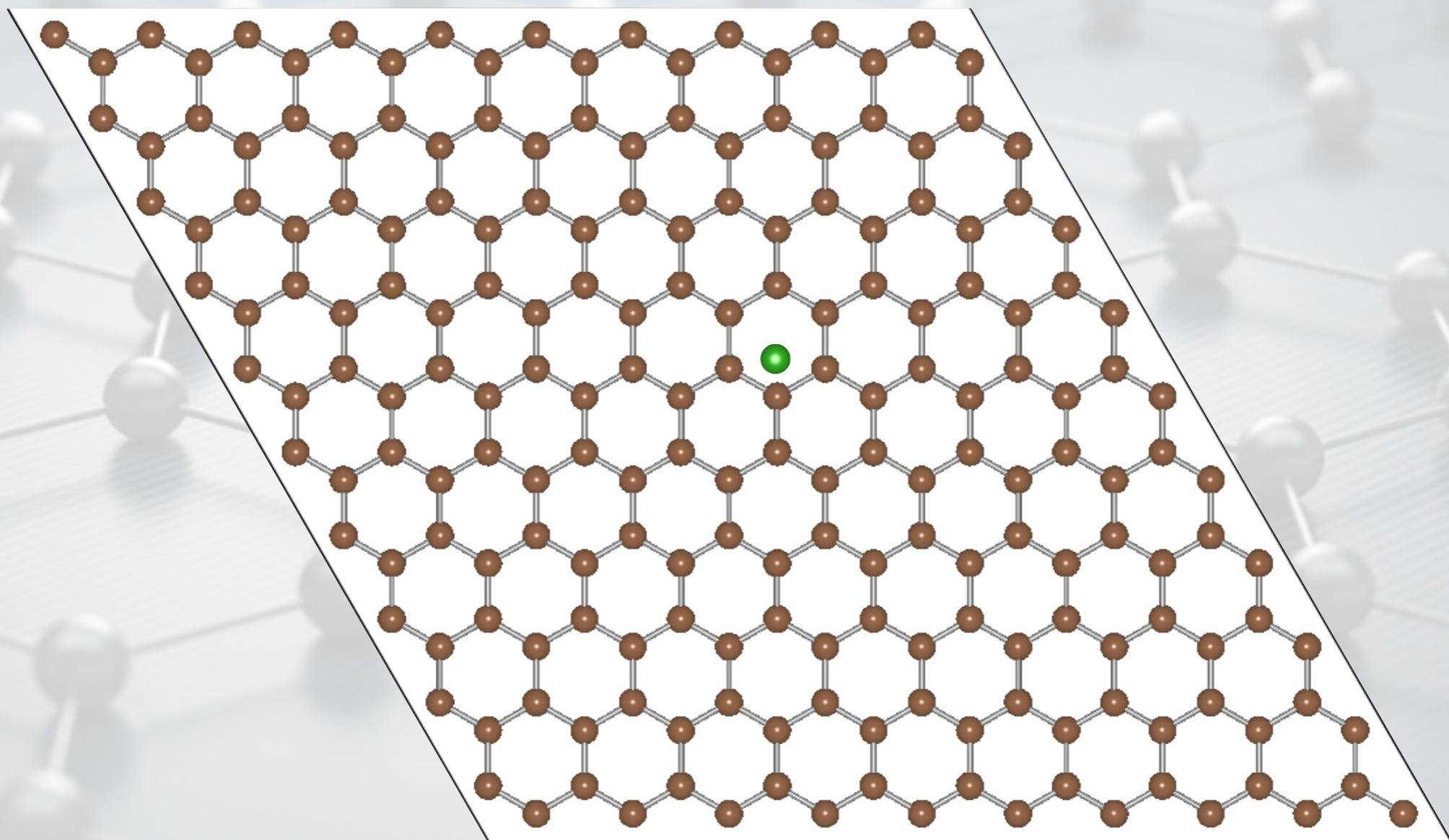
Boron adatoms on graphene



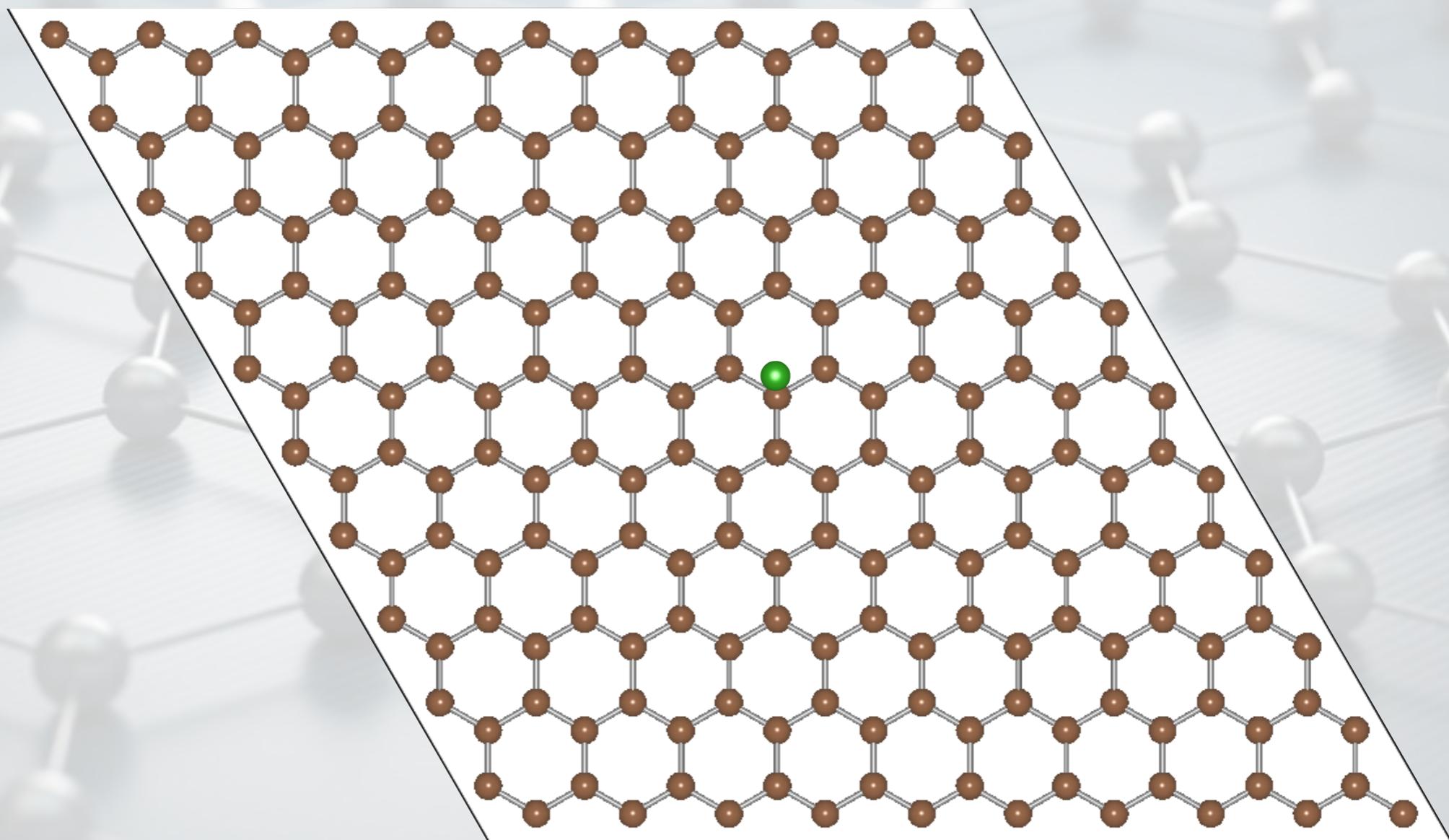
Boron adatoms on graphene



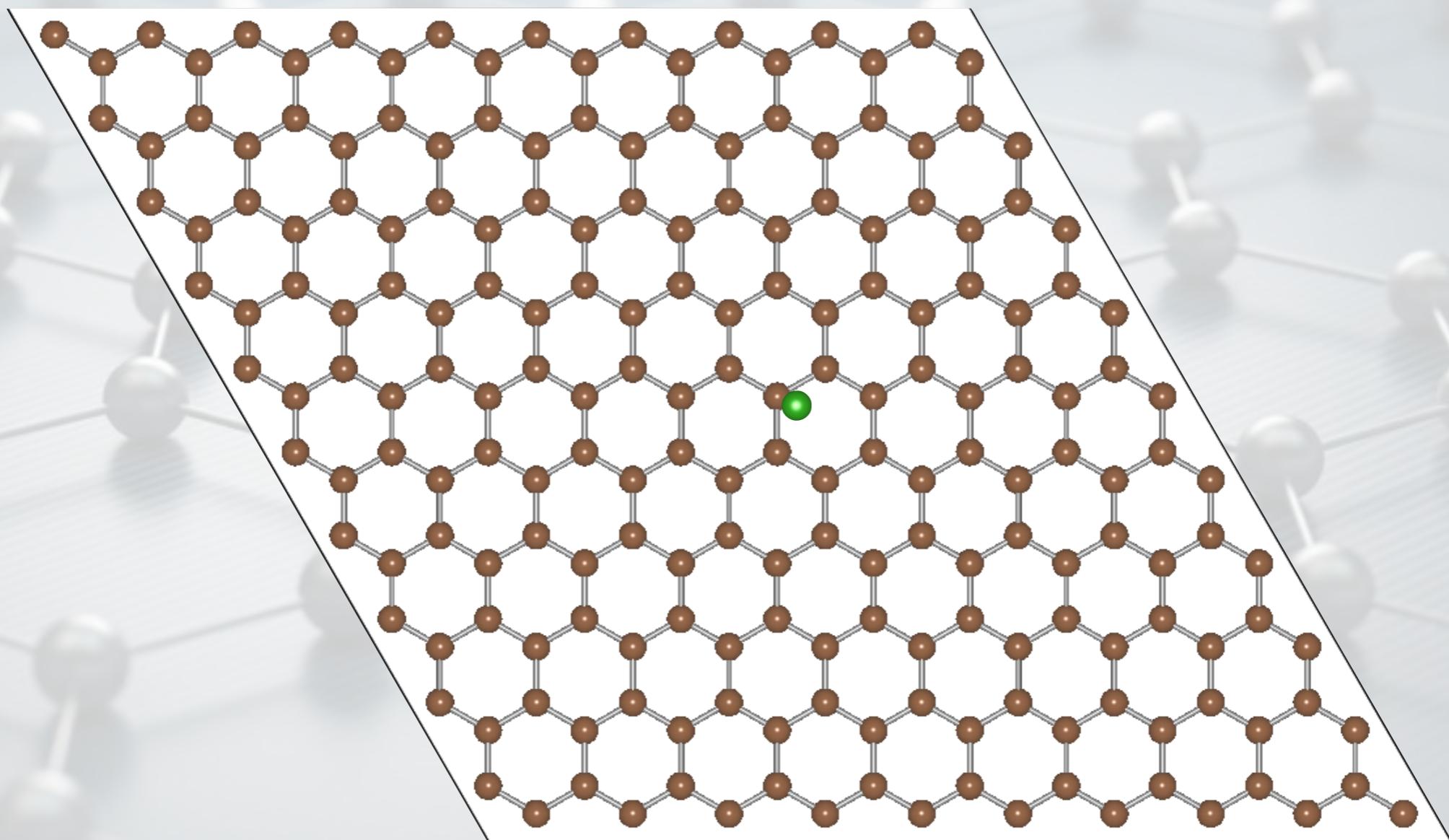
Boron adatoms on graphene



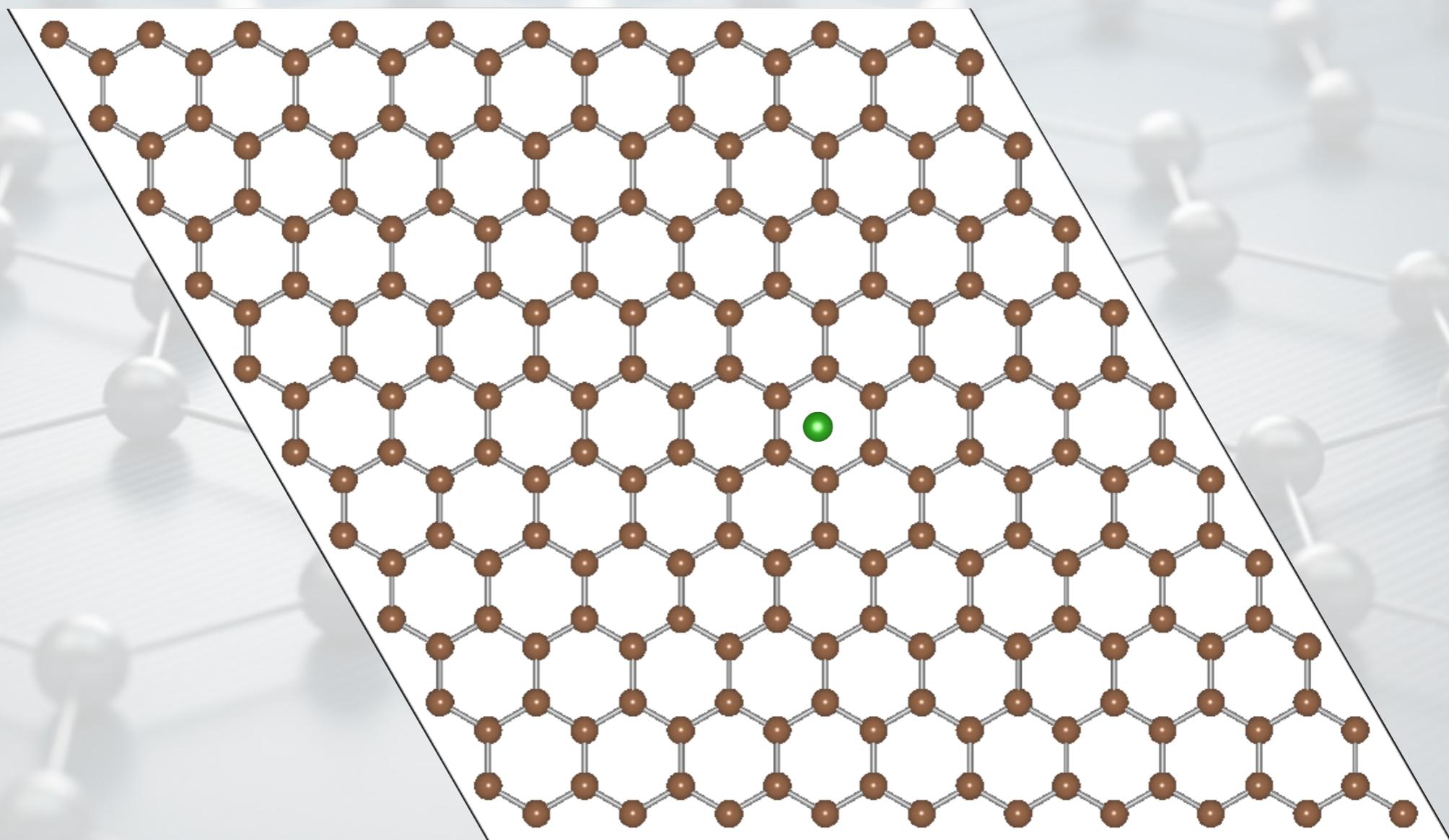
Boron adatoms on graphene



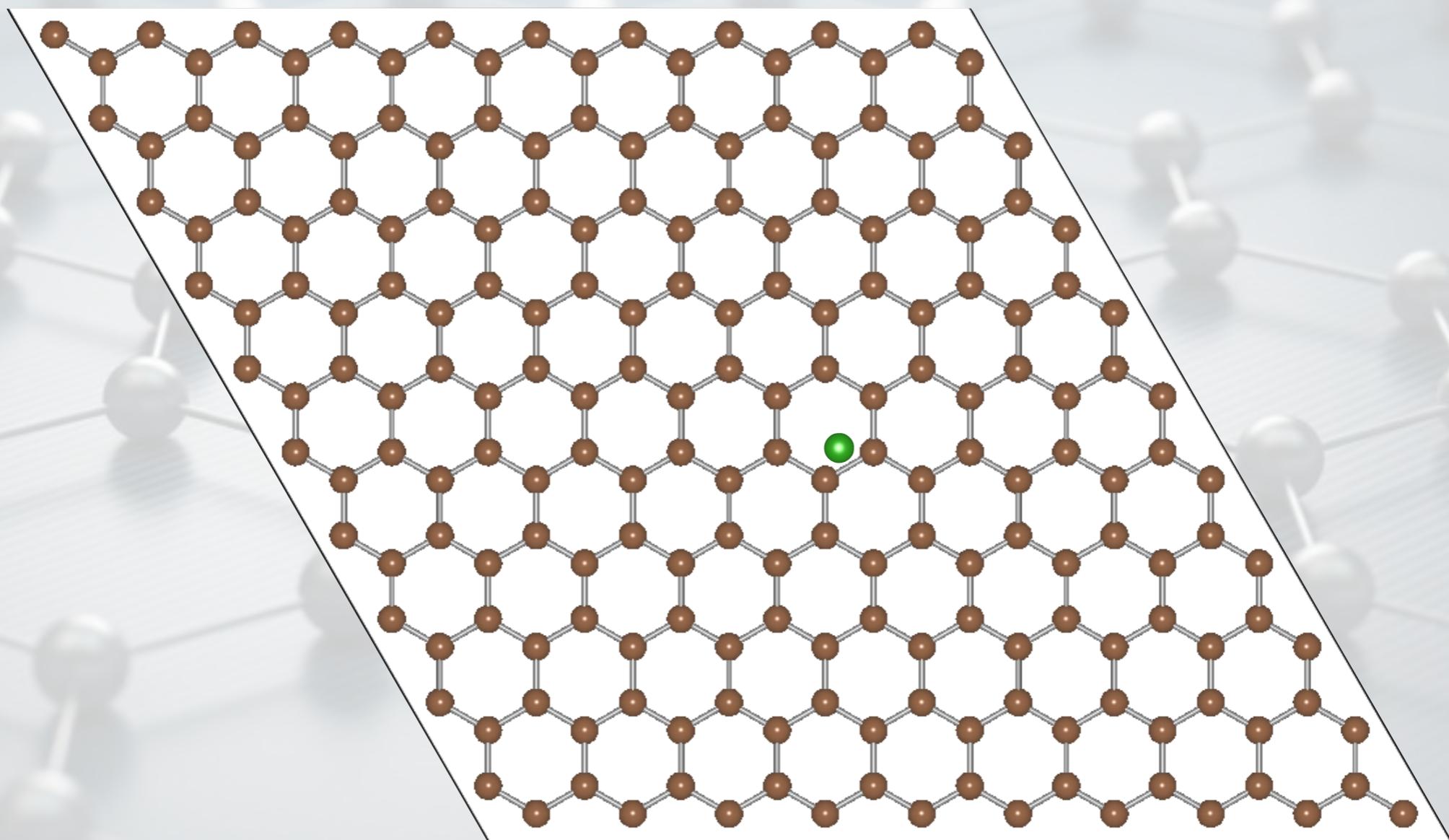
Boron adatoms on graphene



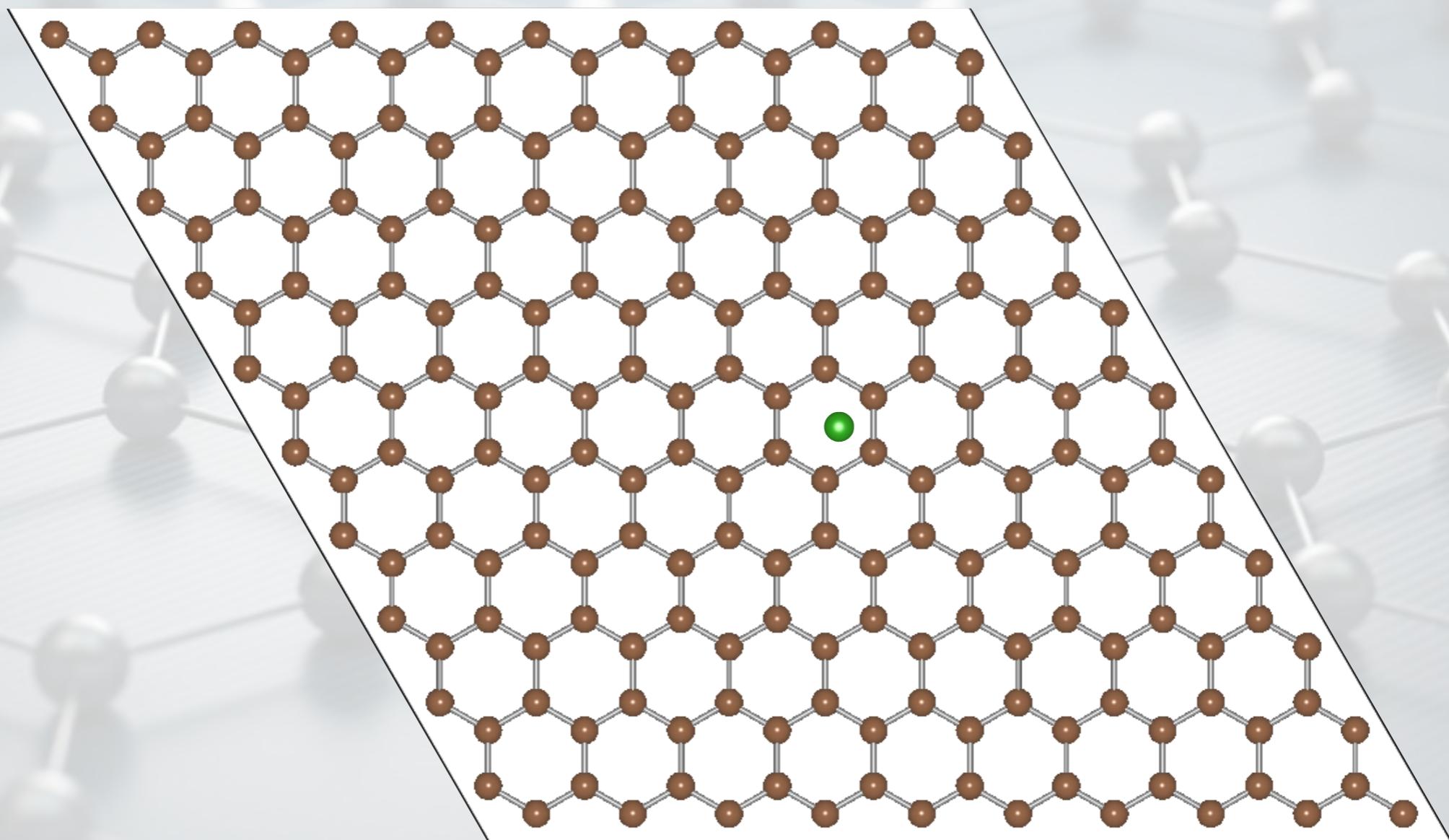
Boron adatoms on graphene



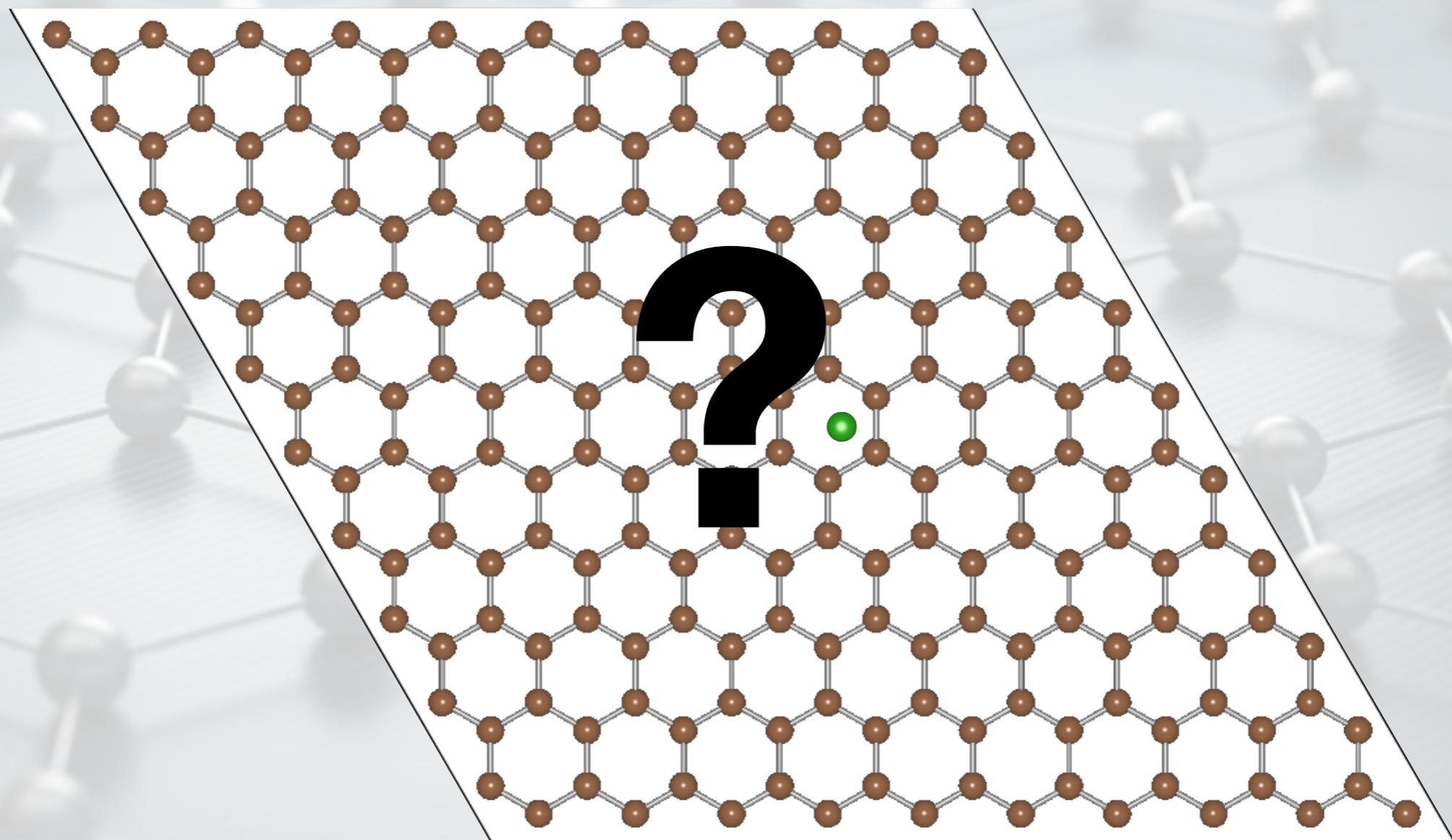
Boron adatoms on graphene



Boron adatoms on graphene



Boron adatoms on graphene



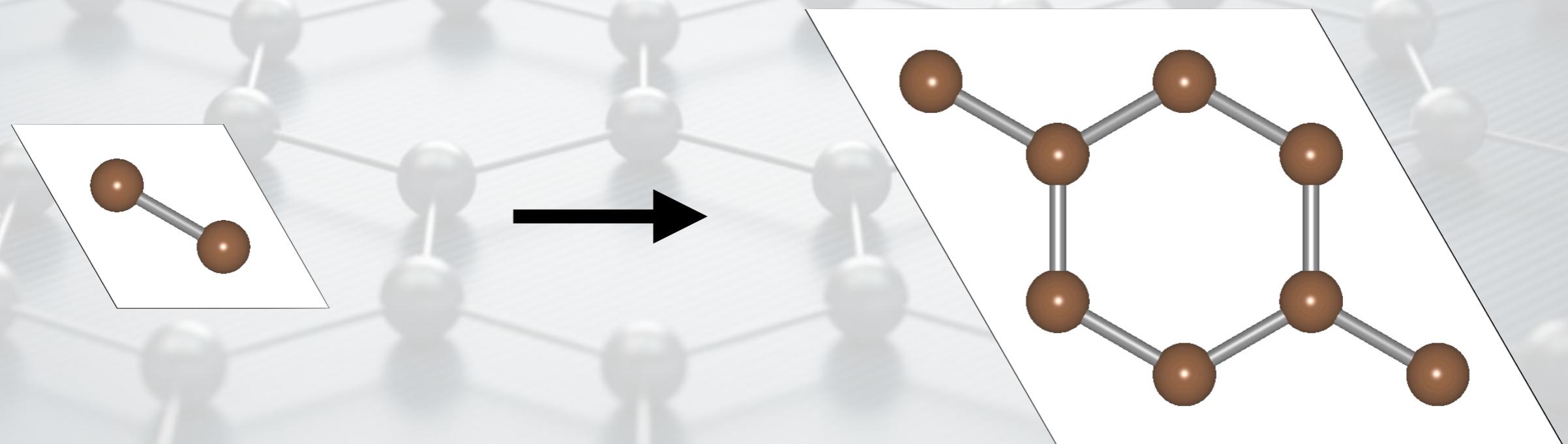
Boron adatoms on graphene



Supercell

Primitive Cell

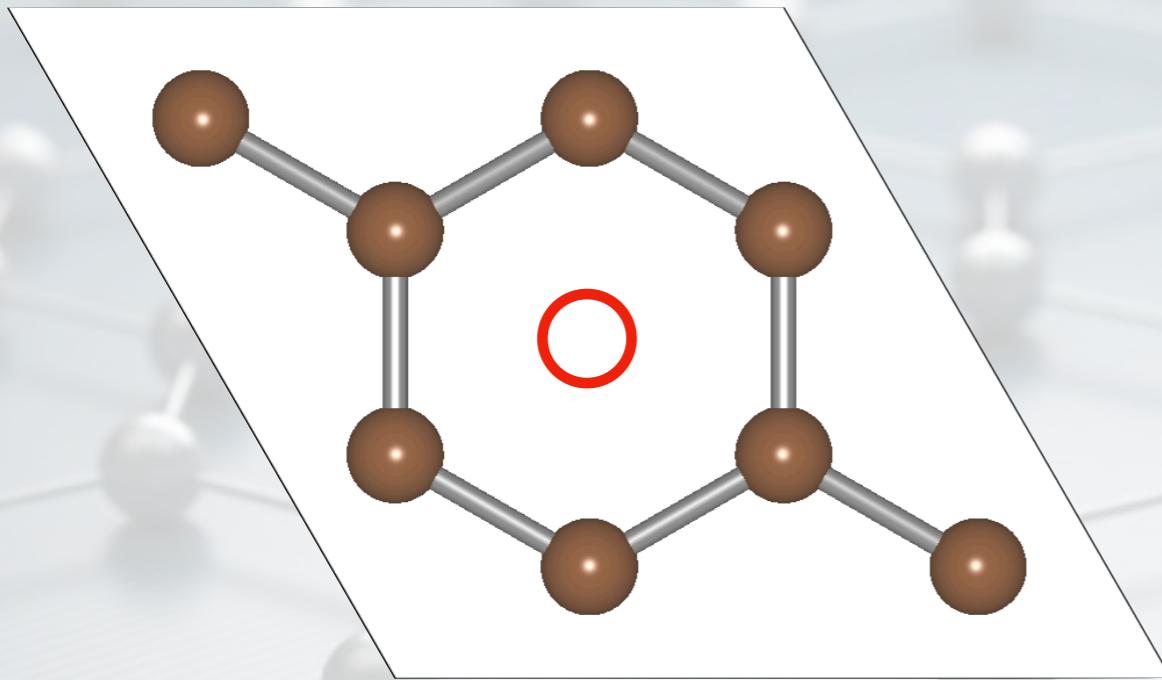
2x2 Supercell



Boron adatoms on graphene



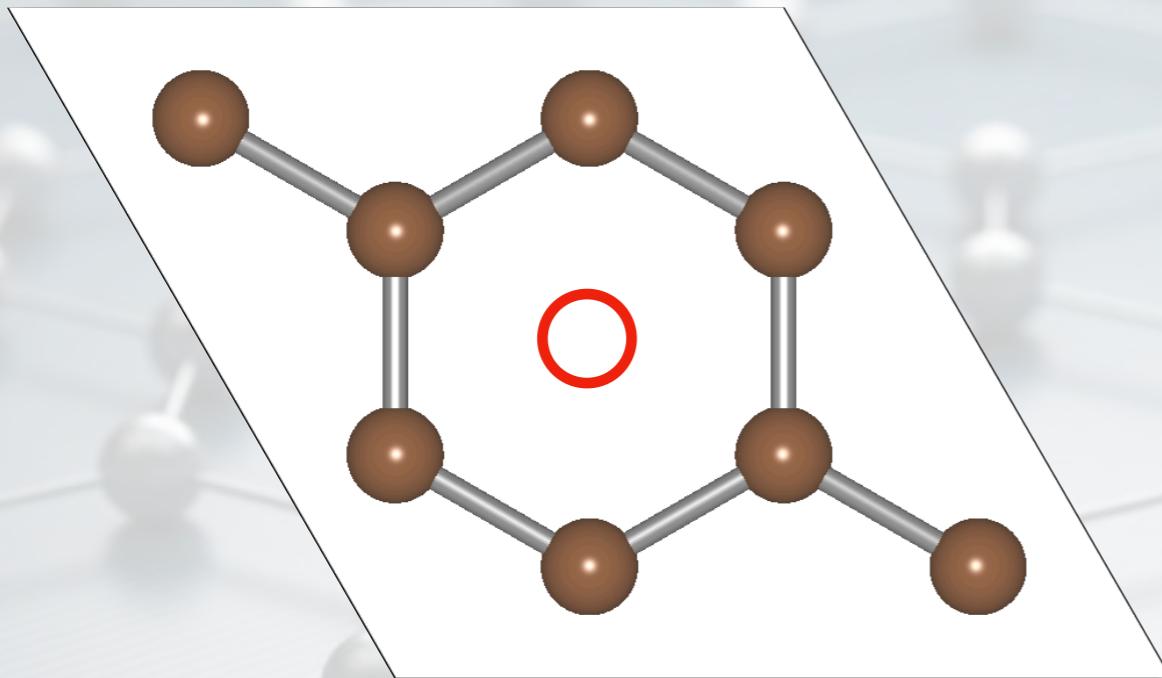
Hollow



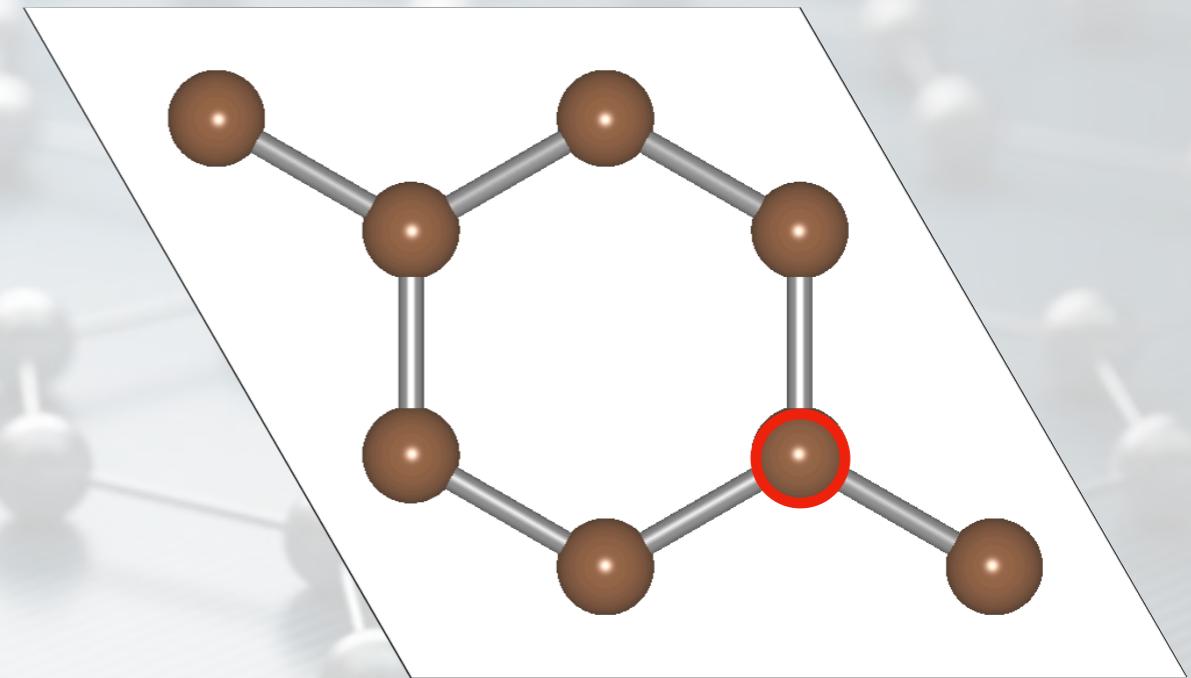


Boron adatoms on graphene

Hollow



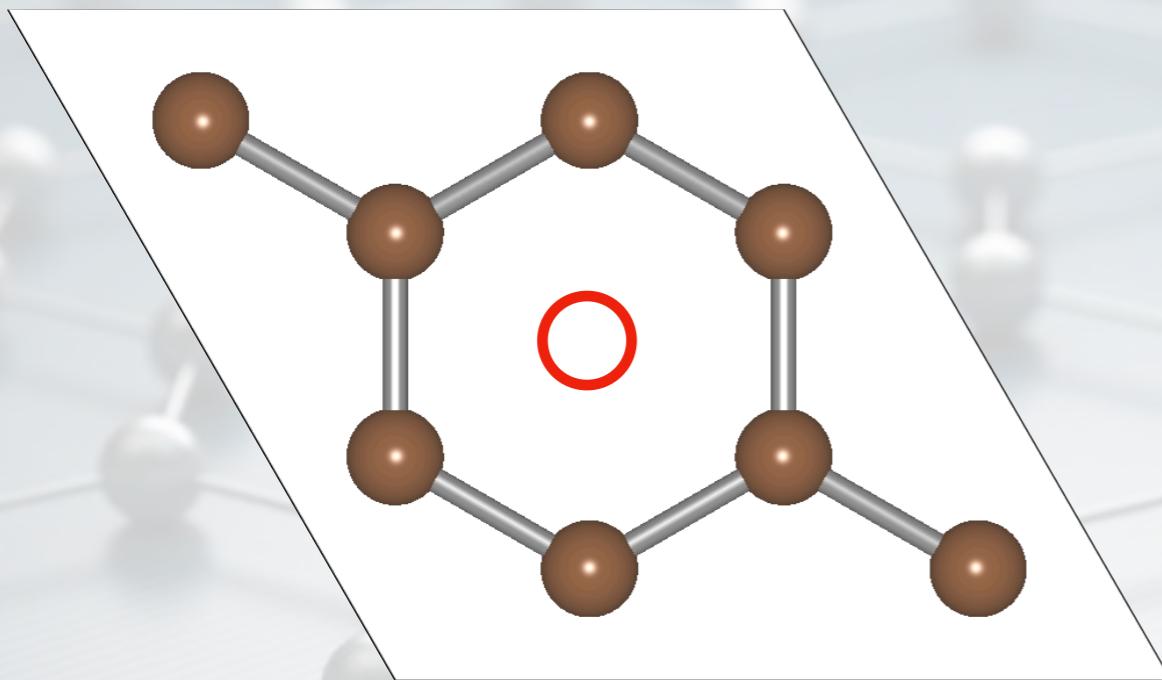
Top



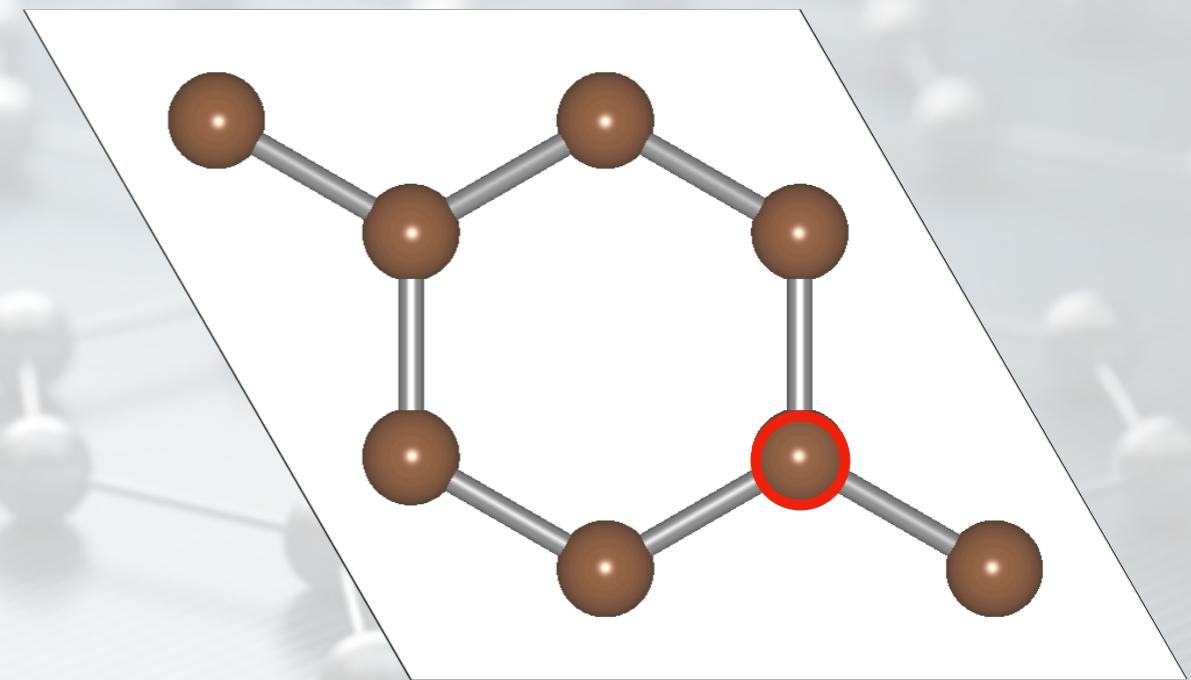


Boron adatoms on graphene

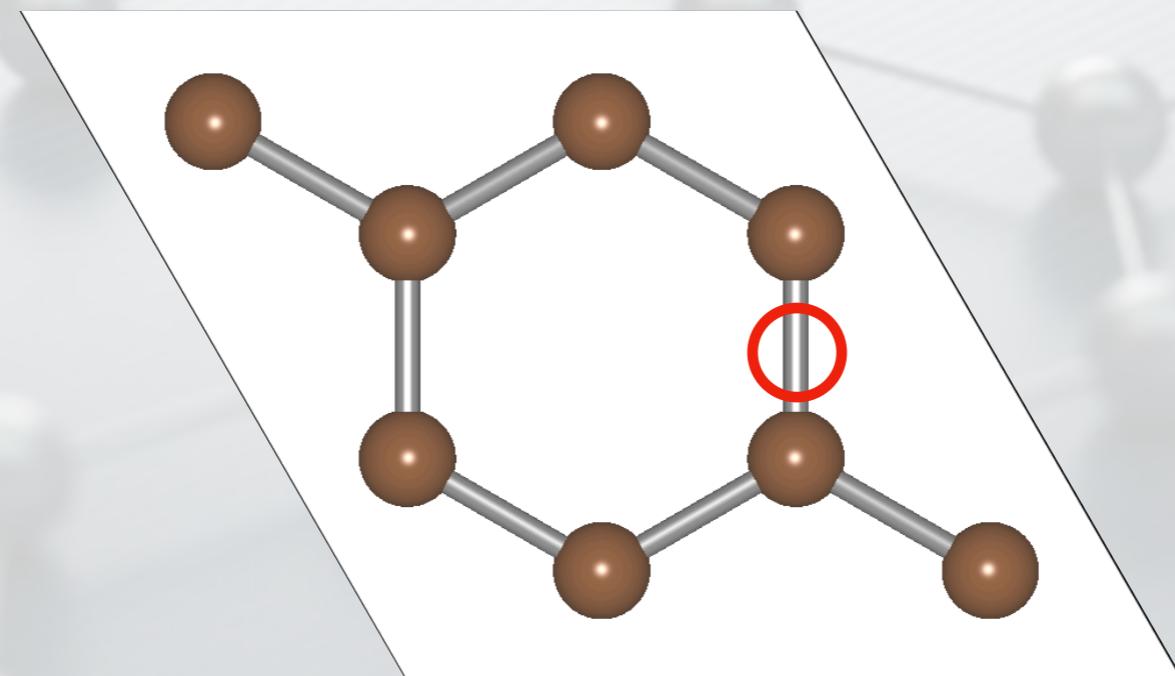
Hollow



Top



Bridge



Boron adatoms on graphene



Hollow

Top

**Finite-size correction scheme for
supercell calculations in Dirac-point
two-dimensional materials**

C. G. Rocha ^{1,2,3}, A. R. Rocha ^{4,5}, P. Venezuela⁶, J. H. Garcia ^{7,8} & M. S. Ferreira^{1,2,3}

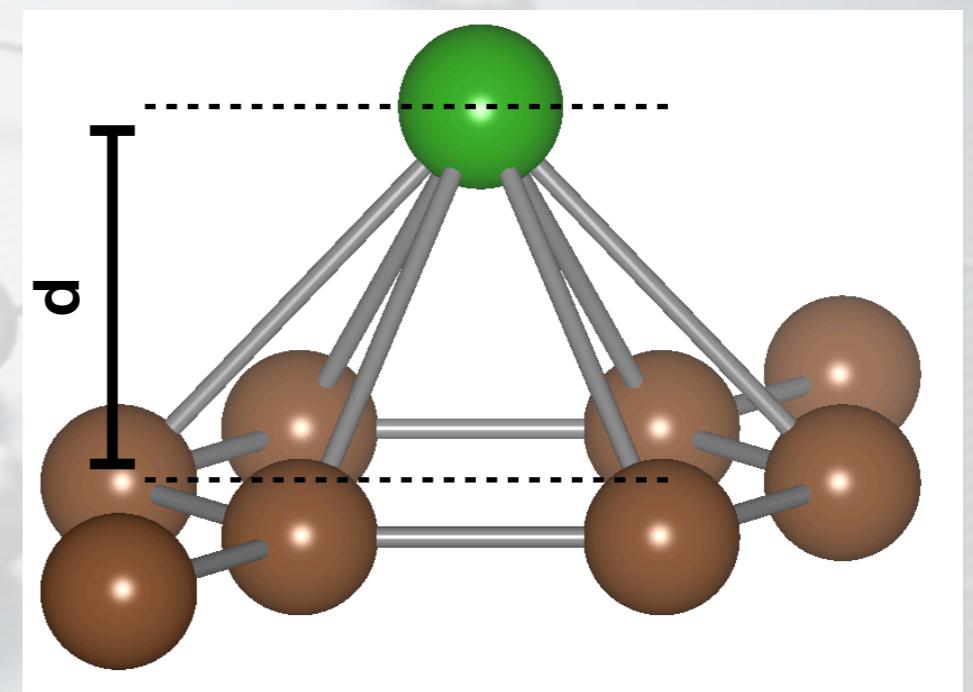
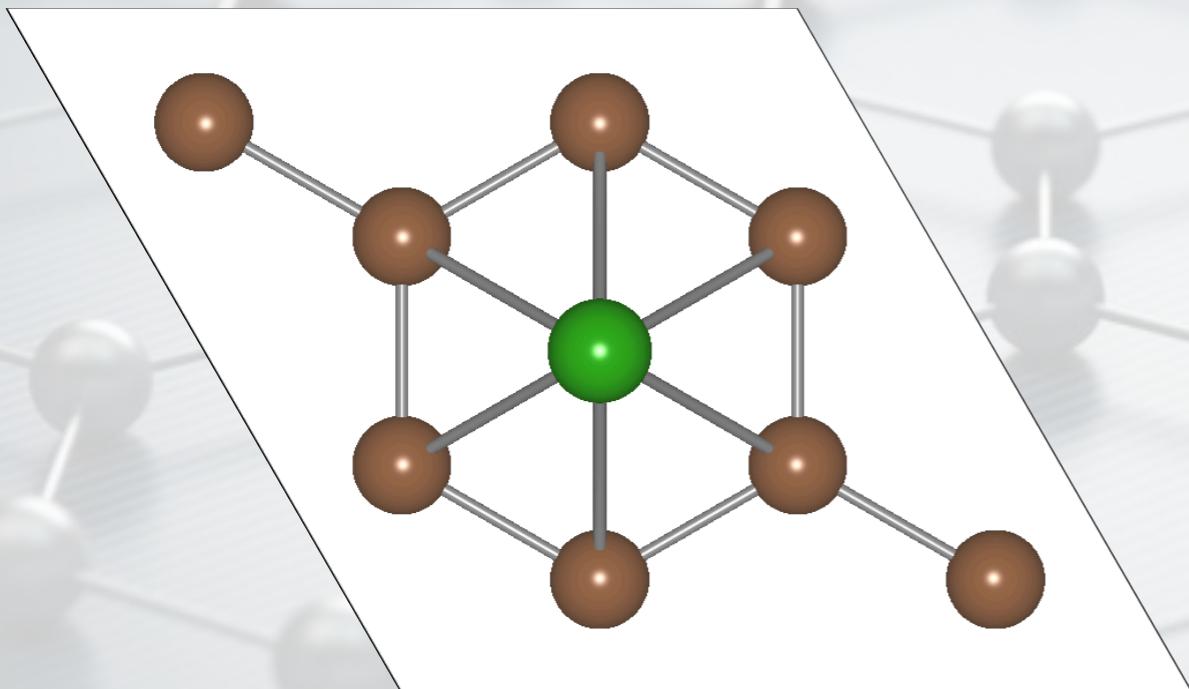
SCIENTIFIC REPORTS | (2018) 8:9348 | DOI:10.1038/s41598-018-27632-6



Boron adatoms on graphene

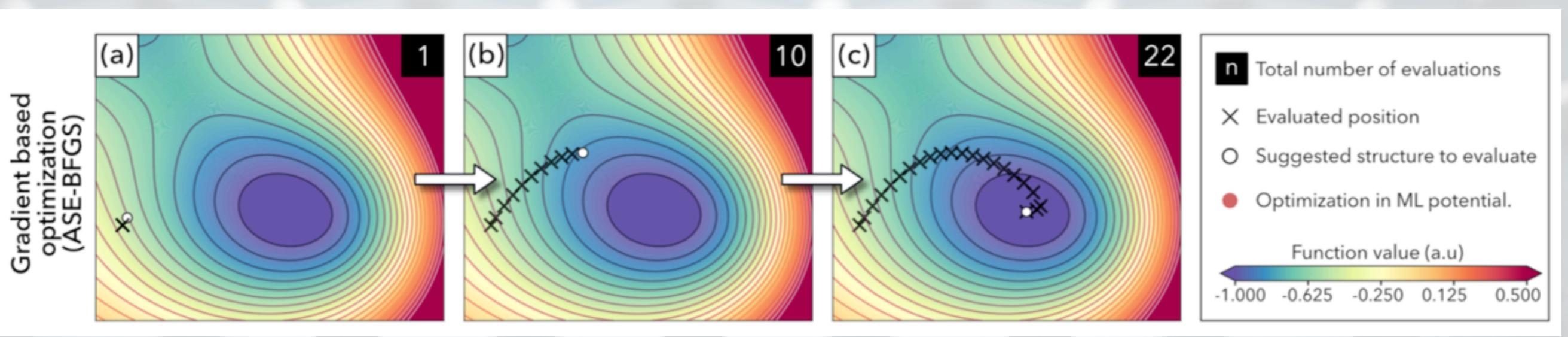


Hollow





Boron adatoms on graphene





Boron adatoms on graphene

(a) 1 (b) 10 (c) 22 n Total number of evaluations

ion_dynamics **CHARACTER**

Specify the type of ionic dynamics.

For different type of calculation different possibilities are allowed and different default values apply:

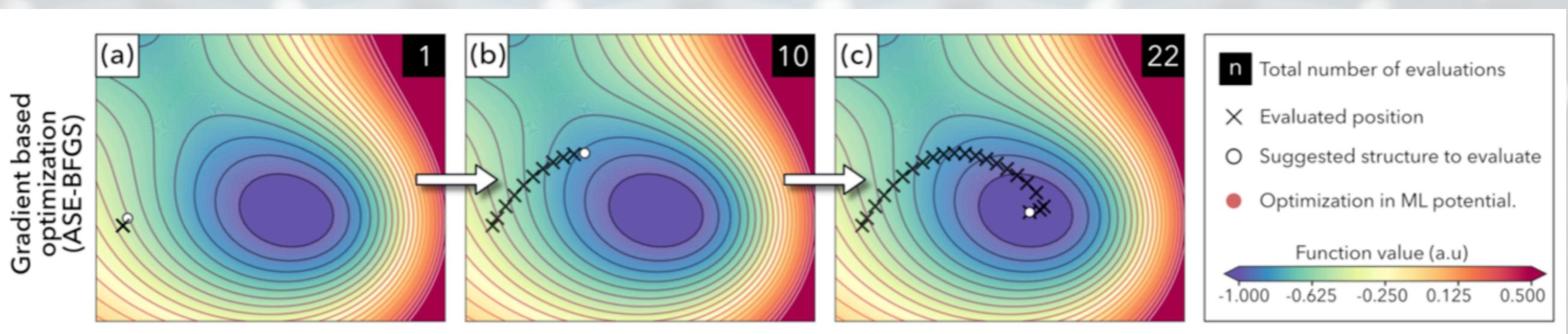
```
CASE ( calculation == 'relax' )

'bfgs' :
  (default) use BFGS quasi-newton algorithm,
  based on the trust radius procedure,
  for structural relaxation

'damp' :
  use damped (quick-min Verlet)
  dynamics for structural relaxation
  Can be used for constrained
  optimisation: see CONSTRAINTS card
```



Boron adatoms on graphene



Boron adatoms on graphene



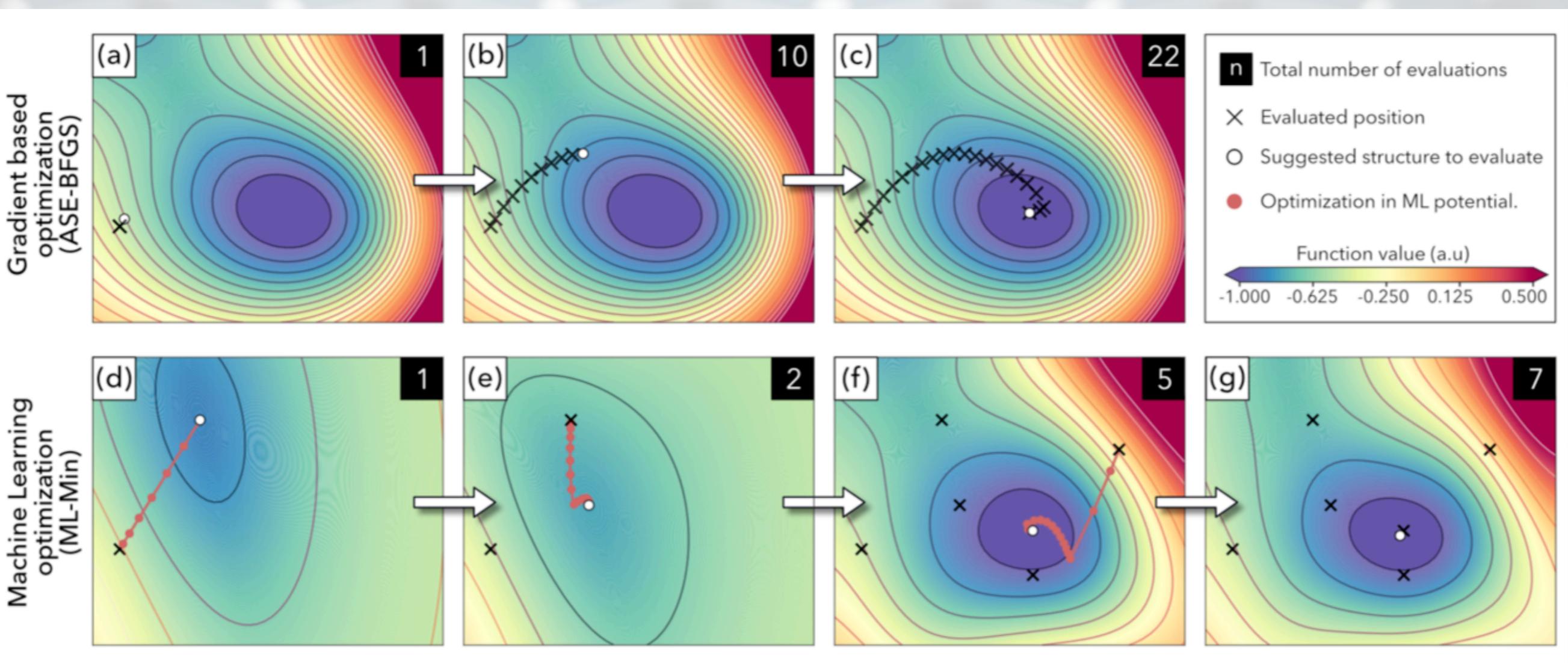
An Atomistic Machine Learning Package for Surface Science and Catalysis

Martin Hangaard Hansen,^{†,‡} Jose Antonio Garrido Torres,^{†,‡} Paul C. Jennings,^{†,‡}

Ziyun Wang,^{†,‡} Jacob Russell Boes,^{†,‡} Osman G. Mamun,^{†,‡} and Thomas

Bligaard^{*,†,‡}

Boron adatoms on graphene



Boron adatoms on graphene



- Which is the most favorable adsorption site
- Binding energy
- How does Boron changes graphene's electronic properties?