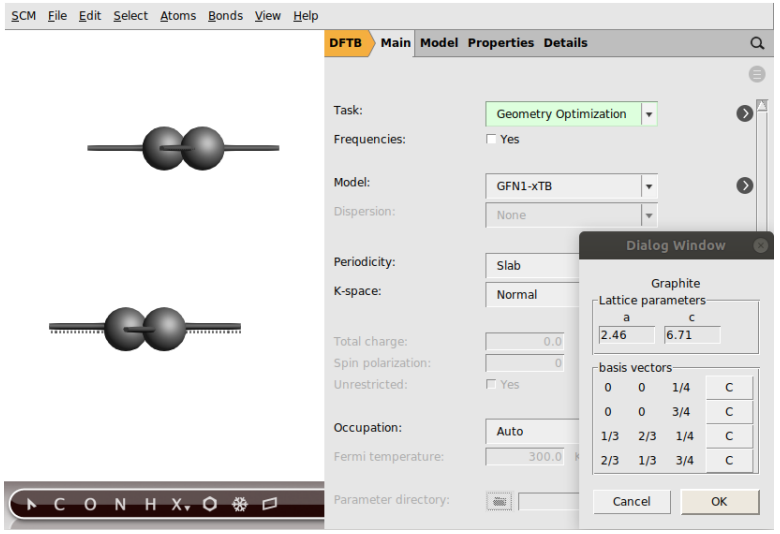
Periodic Structures

- File → Import Coordinates → cif/POSCAR/xyz
  - SCM extended xyz-format

```
3

O       5.38944814       4.97842943       5.08087025
H       5.44702552       5.93631265       5.10815739
H       5.21671599       4.69375471       4.18046817
VEC1      10.00000000        0.00000000        0.00000000
VEC2       0.00000000       10.00000000        0.00000000
VEC3       0.00000000        0.00000000       10.00000000
```

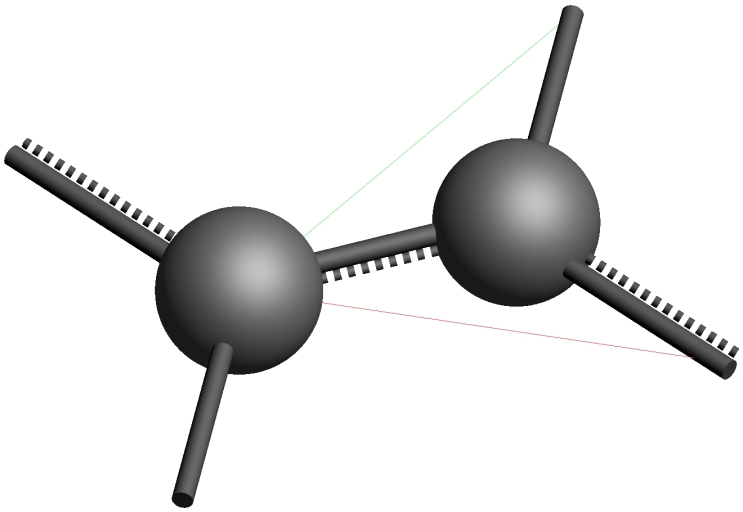
- Common structures from library
  - Switch to periodic engine e.g. ADF → DFTB
  - Periodicity → Bulk
  - Crystal structure library:
    
    → Hexagonal → Graphite



Slab Models for Surfaces

- Manually: **Periodicity → Slab**
- Create surface
  - **Edit → Crystal → Generate Slab**
  - Set Miller indices. Here: **0 0 1**
  - Number of layers: **1**
- Select and delete one carbon layer

Tip: use hotkeys **ctrl + 1**, **ctrl + 2**, **ctrl + 3** to switch perspectives



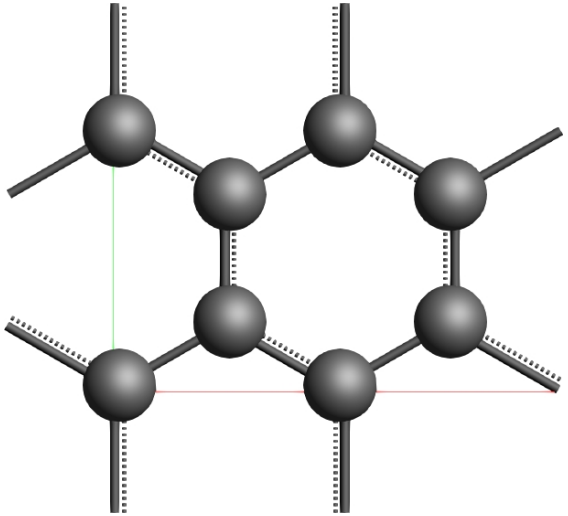
Tip: **Edit → Crystal**
→ Map Atoms to (0 .. 1)

Lattice Optimization

- Consistent geometry: needs lattice optimization (using GFN-xTB here)
  - **Task → Geometry Optimization**
  - Further Geometry Optimization details: click on 
  - **Optimize Lattice** → tick □ **Yes**
- Save and run calculation: **File → Run**
- Switch to amsmovie to check optimization: **SCM → Movie**
- After calculation, use structure directly in new calculation

Supercells

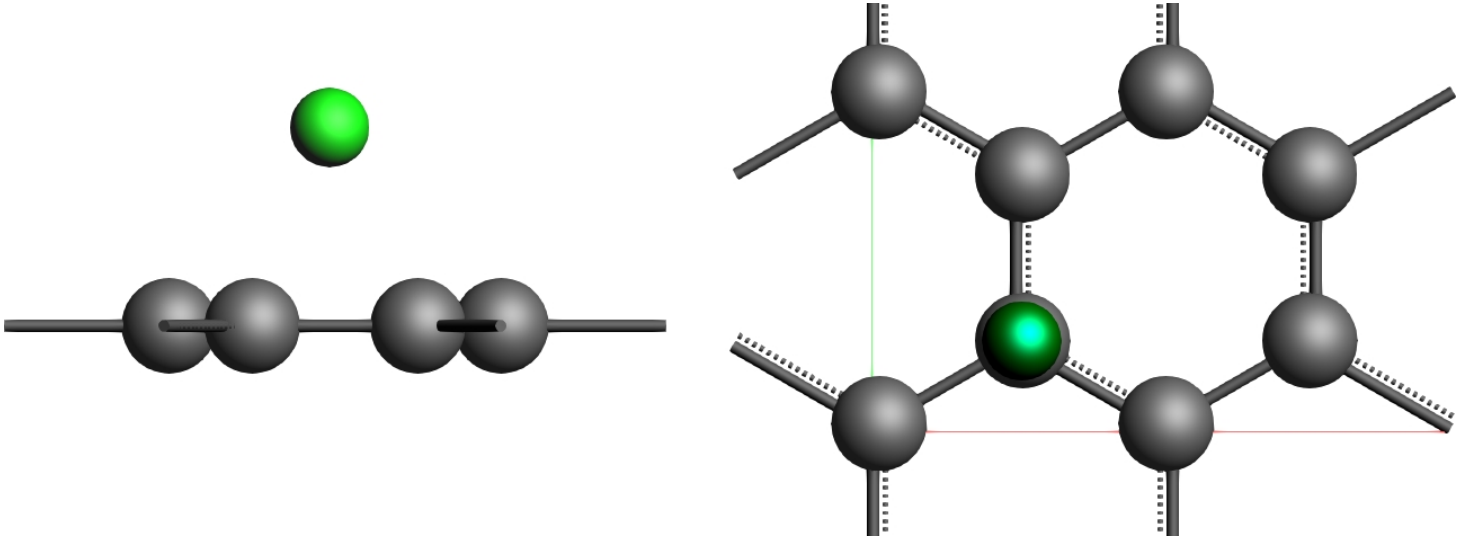
- Adsorption needs a bigger unit cell
  - Edit → Crystal → Generate Super Cell..
  - Enter coefficients 2 0 and -1 2 in popup mask for rectangular cell



- Export Coordinates → .xyz and save for later

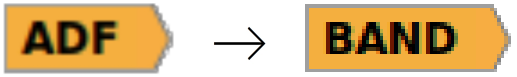
Adsorption Complex

- Click  and select **F** in the periodic table
- Place F-atom on top of Graphene layer, above a C-atom



- Task → Geometry Optimization →  → Disable lattice optimization
- Run optimization, load structure into input afterwards
- **Export Coordinates → .xyz** and save for later

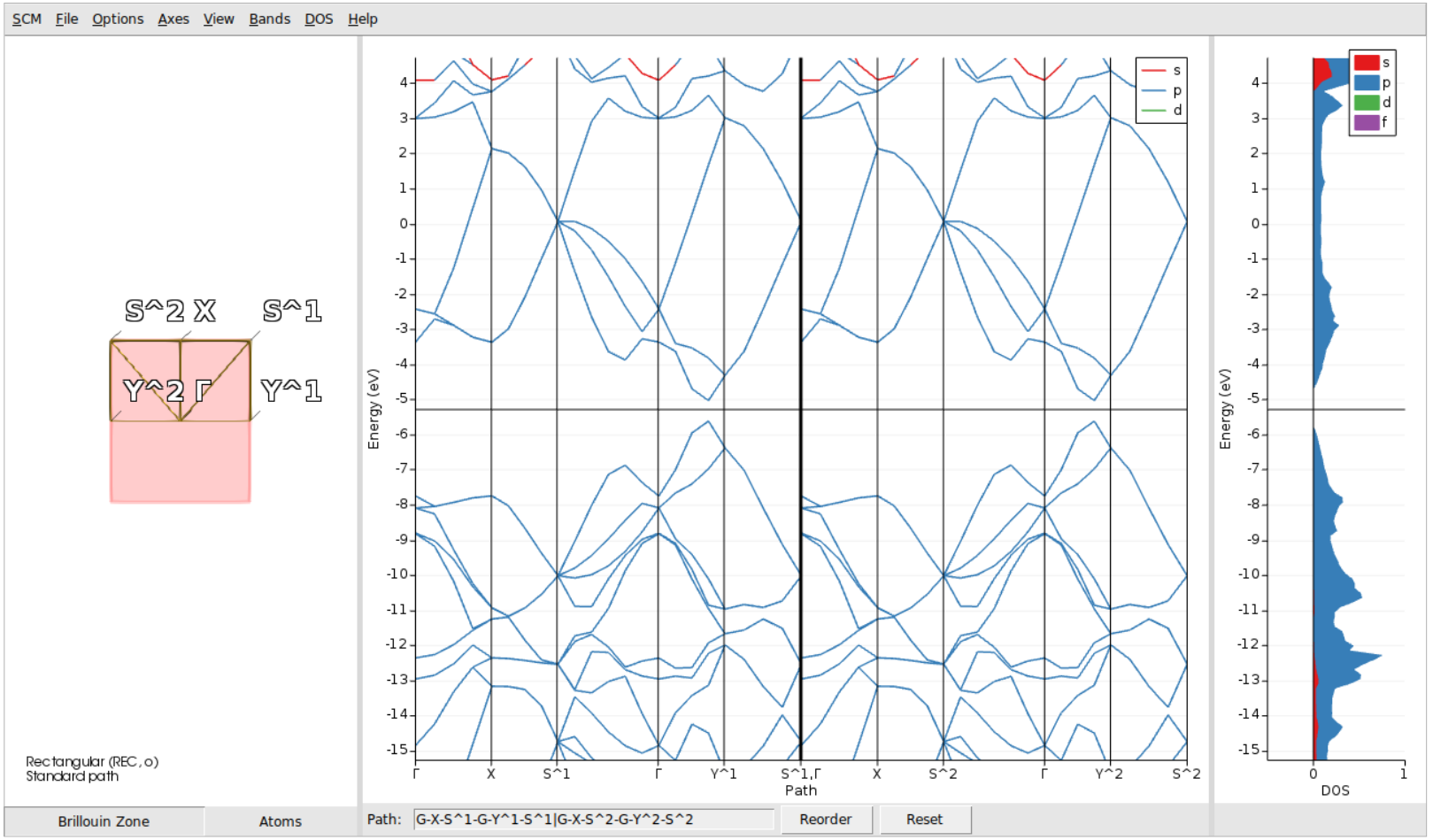
DFT Calculations for DOS & Band Structure

- Open new input
- **File → Import Coordinates** to load adsorption complex geometry
- Switch to BAND 

- **Task → Single Point**
- **Calculate DOS →** tick □ **Yes**
  Calculate band structure → tick □ **Yes**
- Run calculation
- Repeat for Graphene Supercell structure

DOS & Band Structure

- SCM → **band structure** to visualize results



DOS & Band Structure

- projected DOS
  - Switch to **Atoms** view and select atom(s)
  - Right-click on selection and pick the orbitals of interest