Amsterdam Modeling Suite

SCM

ADF

BAND

DFTB

MOPAC

ReaxFF

COSMO-RS

External
Quantum Chemistry Codes

AMS
driver

GUI

PLAMS

Organic Electronics

Materials

Polymers

Oil & Gas

Batteries

Pharma

Spectroscopy

Nanoscience

Catalysis

Inorganic Chemistry

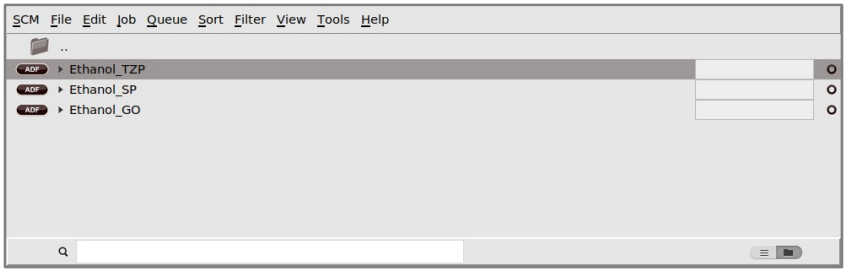
89 Ac

Heavy Elements

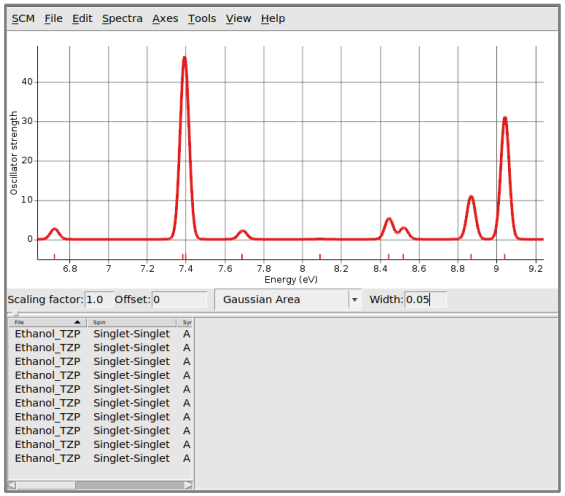
Bonding Analysis

GUI Modules

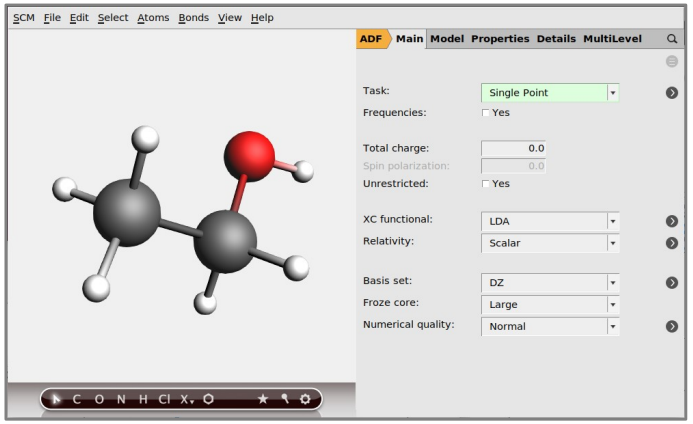
AMSjobs – Calculation Management



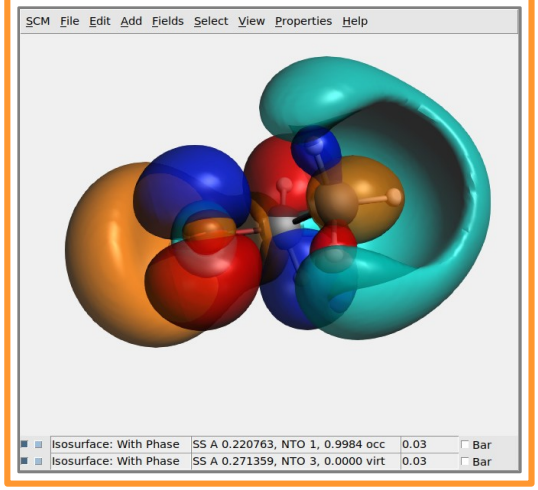
AMSspectra – Spectra



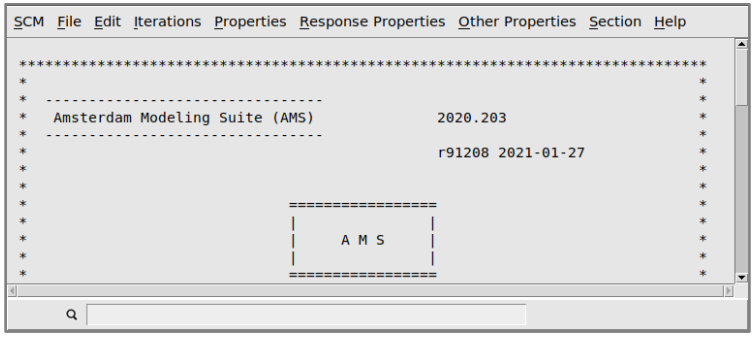
AMSinput – Editor & Settings



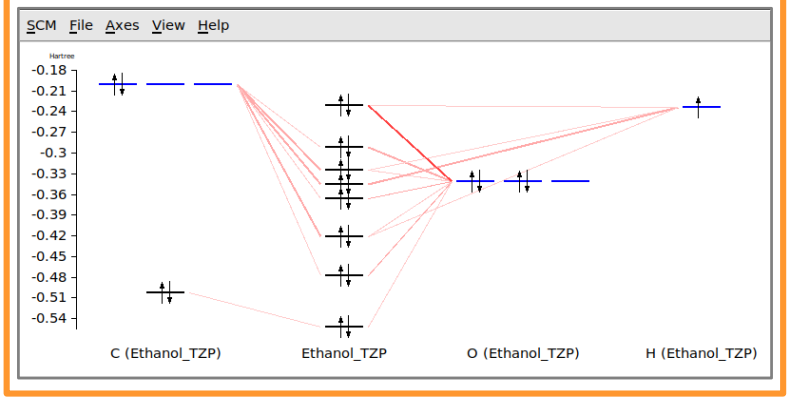
AMSview – 3D Plots



AMSoutput – Text Results



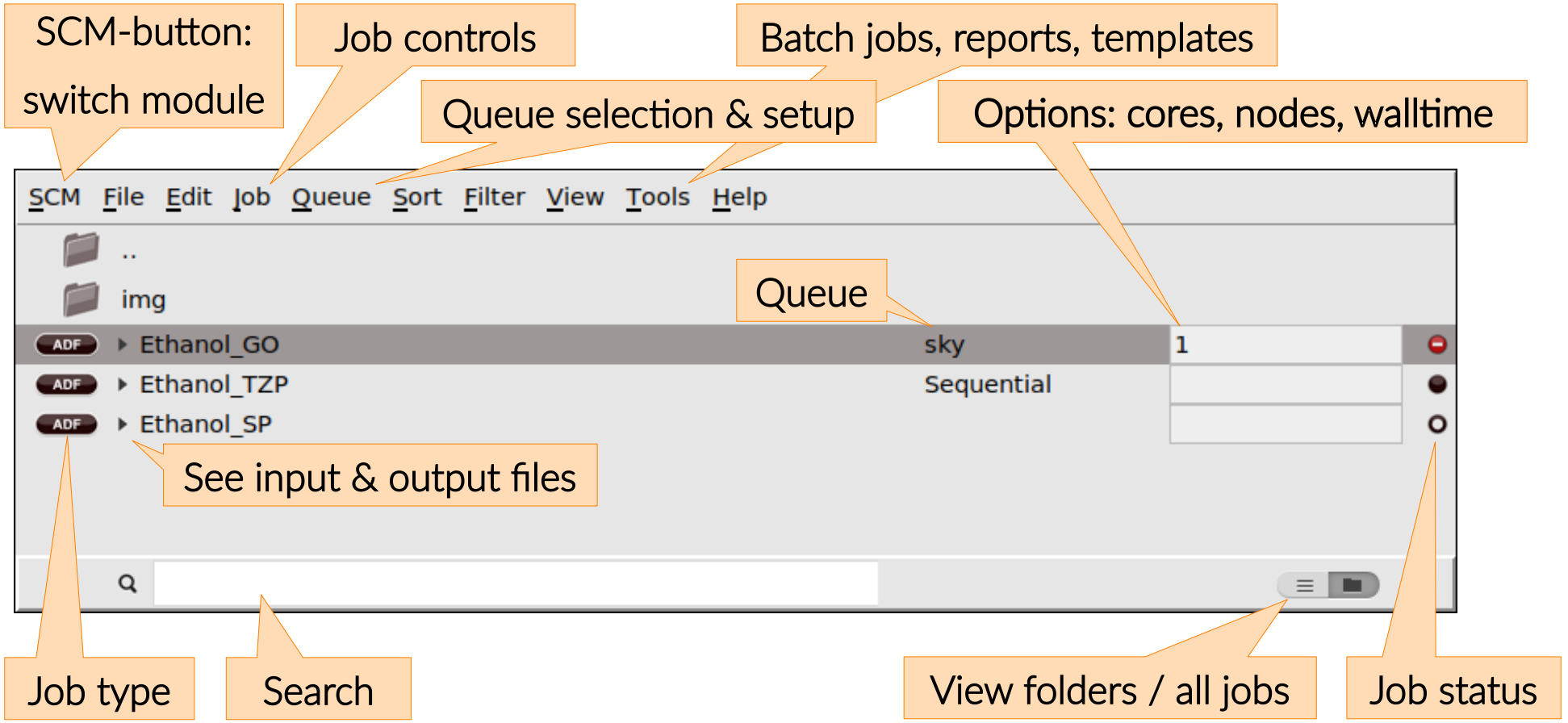
AMSlevels – Orbital Interactions



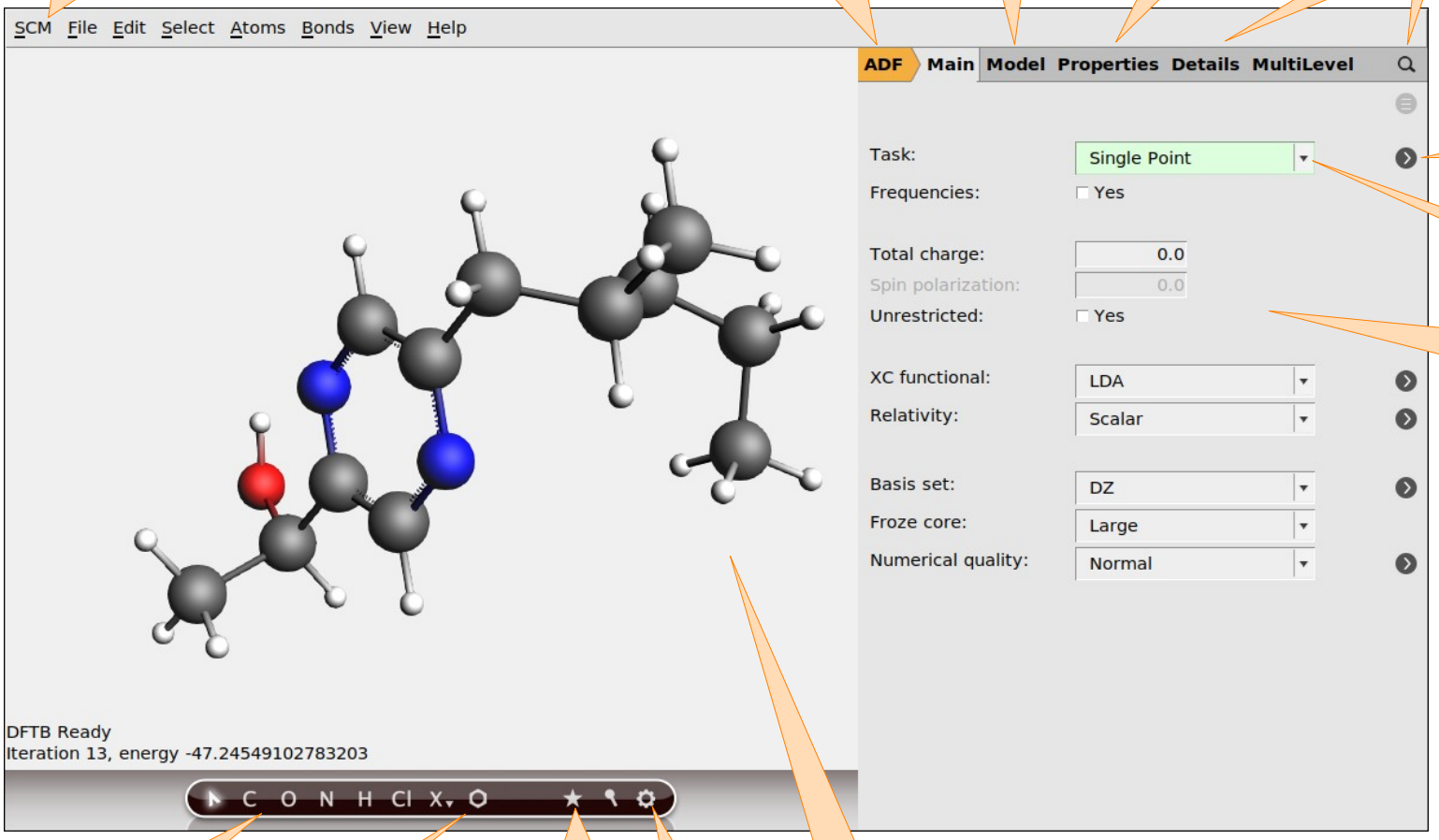
Getting Started

- Open AMSjobs
  - Windows: **`double-click desktop icon`**
  - Mac OSX: **`open Application`**
  - Linux: run **`$ADFBIN/adfjobs`**
- Other GUI modules
  - Open as executables
  - **`SCM-button`** → **`<GUImodule>`**

AMSjobs


SCM-button: switch module
Job controls
Batch jobs, reports, templates
Queue selection & setup
Options: cores, nodes, walltime
SCM File Edit Job Queue Sort Filter View Tools Help
..
img
Queue
ADF Ethanol_GO
sky
1
ADF Ethanol_TZP
Sequential
ADF Ethanol_SP
See input & output files
Job type
Search
View folders / all jobs
Job status

AMSinput



SCM-button: switch module

System & Task details

Search library & manual

Switch engine

Results

Technical settings

Details

Task

Settings panels

Elements

Symmetrize

Molecular editor

Template Structures

Preoptimize

GUI Controls – ADFinput Editor Controls

Free rotation	**left mouse button** (**LMB**) & drag
In-plane rotation	**ctrl** + **LMB** & drag
In-plane shift	**right mouse button** (**RMB**) & drag
Zoom	**mouse wheel** / **alt** & drag
Area selection	**shift** + **LMB**
Deselect	**LMB** on drawing space
Undo	**ctrl** + **Z**
Redo	**shift** + **ctrl** + **Z**
View along x- / y- / z-axis	**ctrl** + **1** / **ctrl** + **2** / **ctrl** + **3**

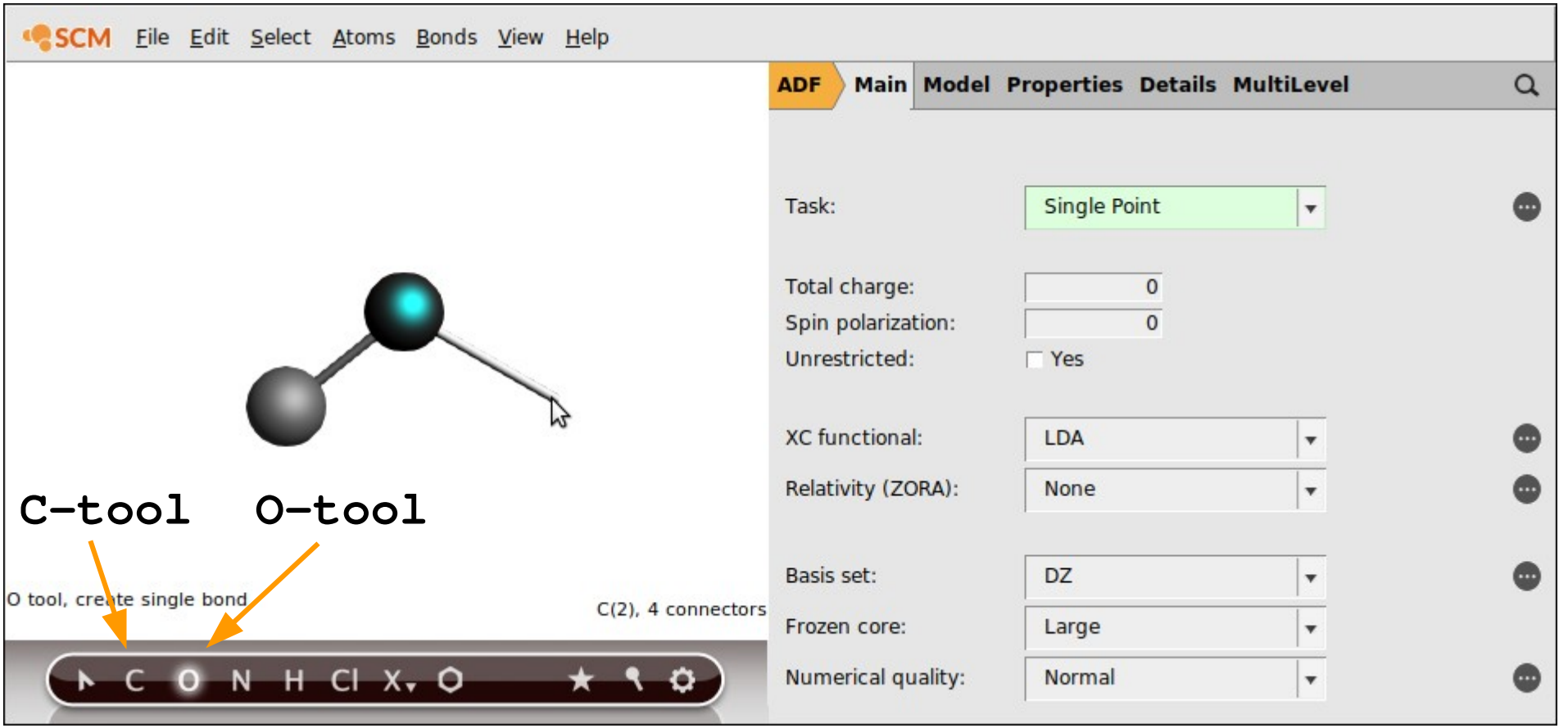
GUI Controls – ADFinput Editor Controls

- Selection free rotation **LMB** & drag from a selected atom
- Selection In-plane rotation **ctrl** + **LMB** & drag from atom
- Selection in-plane shift (**shift** +) **RMB** & drag from atom
- Select all atoms **ctrl** + **A**
- Add hydrogen atoms **ctrl** + **E**
- Link selected atoms **ctrl** + **L**
- Delete selected atoms **del** / **backspace**

- More shortcuts: **Help** → **Shortcuts**

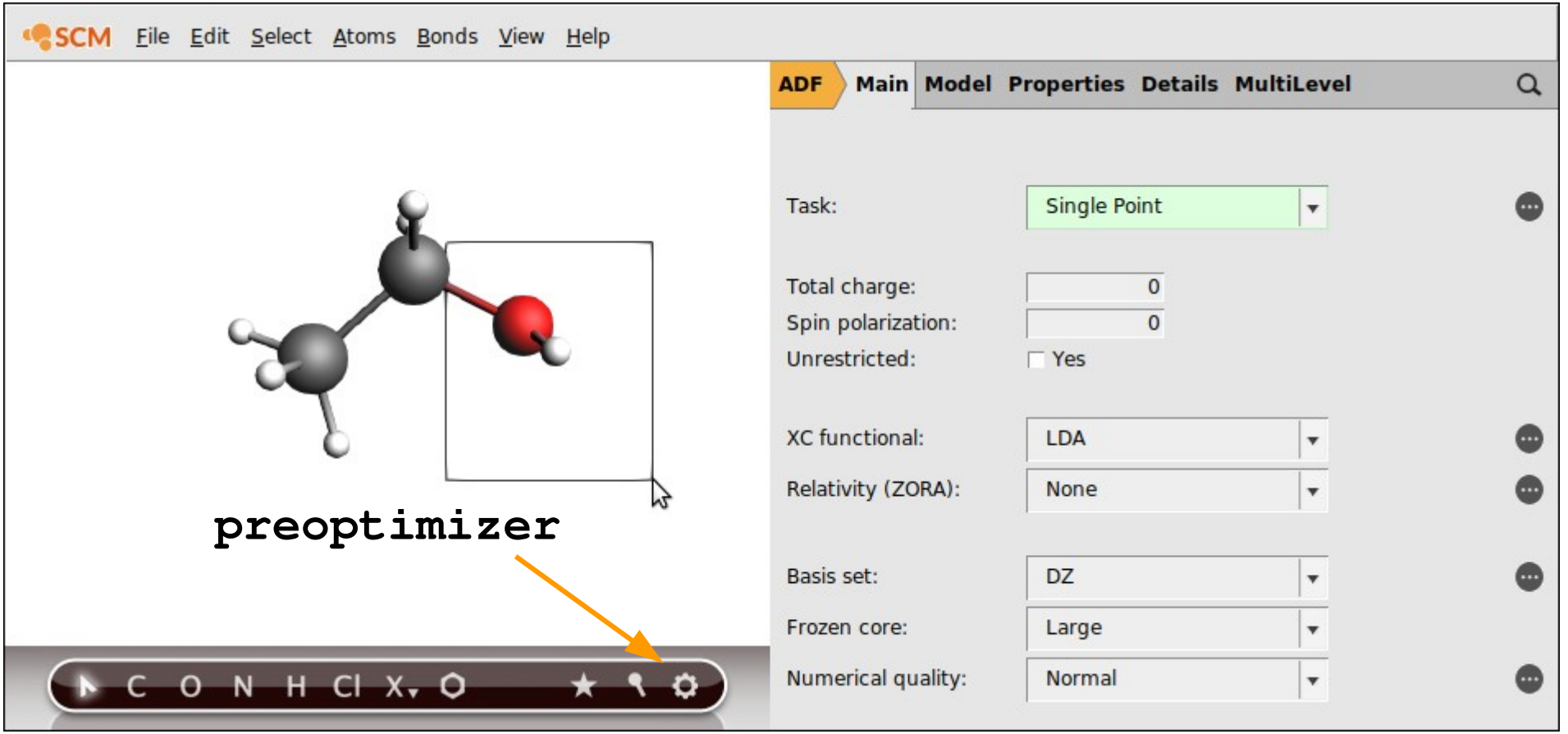
GUI Controls – Molecular Editor

- Click on **`C-tool`** & place first C-atom
- Draw bond & place second C-atom
- Click on **`O-tool`**, draw bond & place O-atom



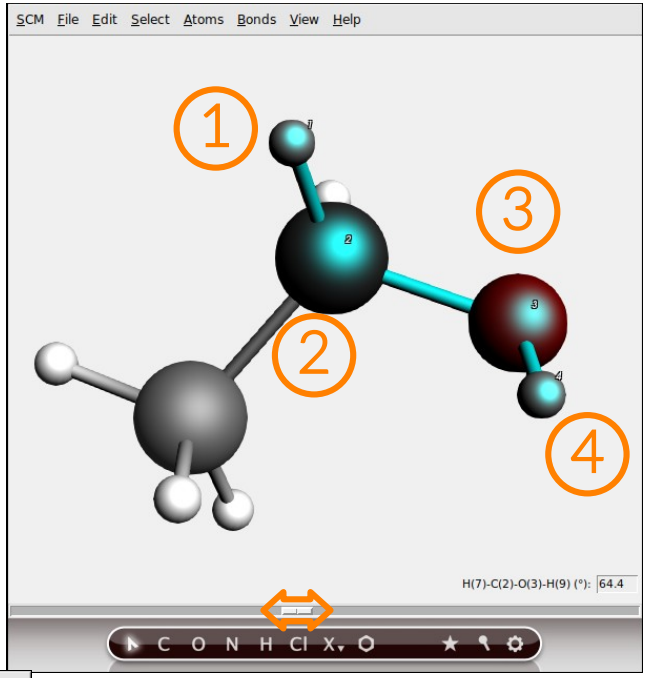
GUI Controls – Molecular Editor

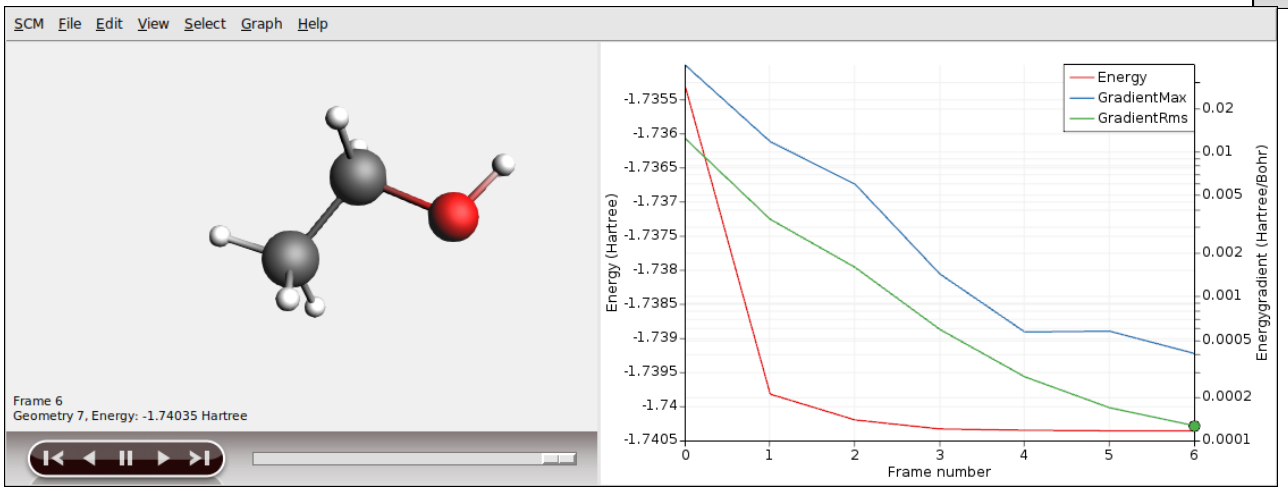
- Leave drawing mode with **esc** & **LMB**
- **ctrl** + **E** to saturate with H-atoms
- Area select (**shift** + **LMB**) OH group
- Rotate OH into anti-conformation & click **preoptimizer** button



Geometry Optimization

- When preoptimization yields wrong conformer
  - Hold **`shift`** & click atoms in order H-C-O-H
  - Set slider on bottom bar to proper angle
- Select **`Task`** → **`Geometry Optimization`**
  - Save & run calculation
  - Monitor progress with **`SCM`** → **`AMSmovie`**

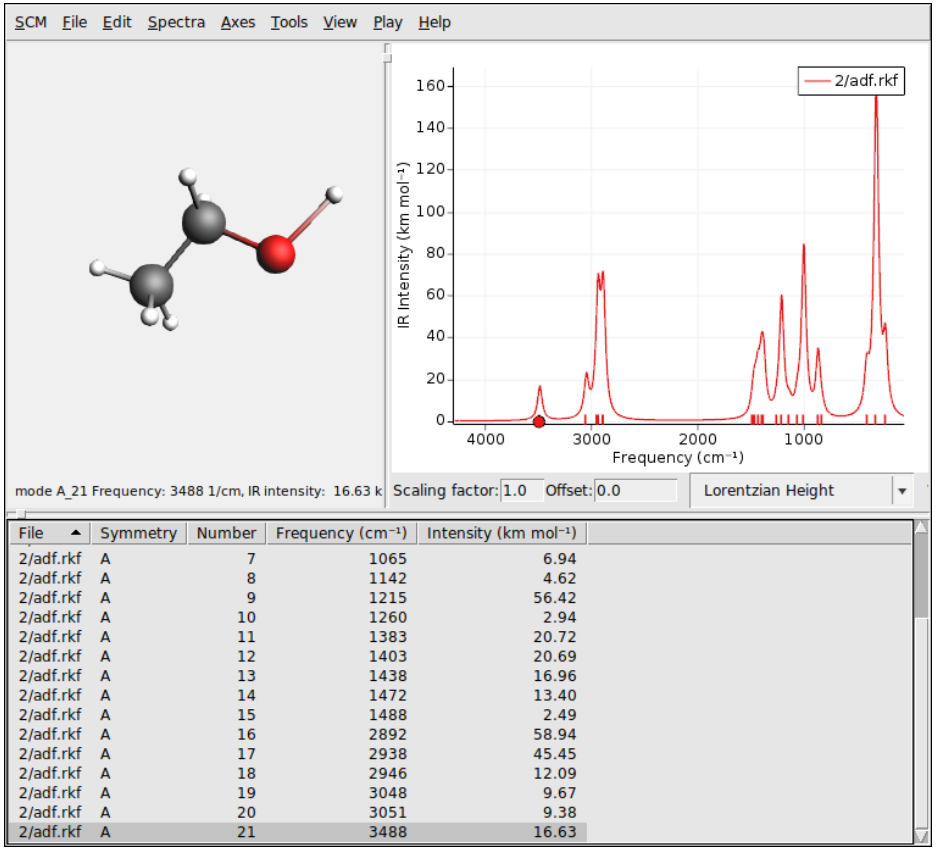




Load Results & Frequency Calculation

- **SCM → New Input**
- Load previously optimized geometry
  - **File → Import Coordinates**
  - Select **<OptimizationJob>.results/ams.rkf**
- **Frequencies:** → tick ☐ **Yes**
- Save & run calculation
- **SCM → Spectra**
  - Examine modes

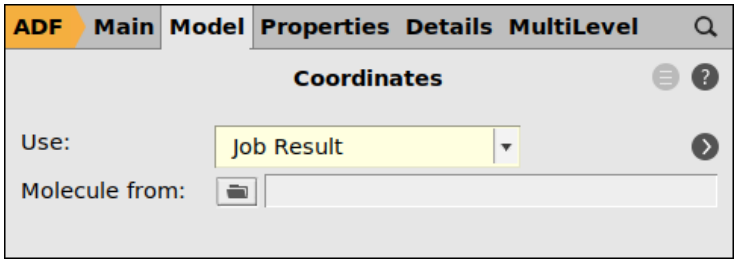
Tip: **ams.rkf** contains driver results (optimization, MD trajectory etc.)
<engine>.rkf contains engine-related data and results



File	Symmetry	Number	Frequency (cm⁻¹)	Intensity (km mol⁻¹)
2/adf.rkf	A	7	1065	6.94
2/adf.rkf	A	8	1142	4.62
2/adf.rkf	A	9	1215	56.42
2/adf.rkf	A	10	1260	2.94
2/adf.rkf	A	11	1383	20.72
2/adf.rkf	A	12	1403	20.69
2/adf.rkf	A	13	1438	16.96
2/adf.rkf	A	14	1472	13.40
2/adf.rkf	A	15	1488	2.49
2/adf.rkf	A	16	2892	58.94
2/adf.rkf	A	17	2938	45.45
2/adf.rkf	A	18	2946	12.09
2/adf.rkf	A	19	3048	9.67
2/adf.rkf	A	20	3051	9.38
2/adf.rkf	A	21	3488	16.63

GUI Efficiency Tricks & Features

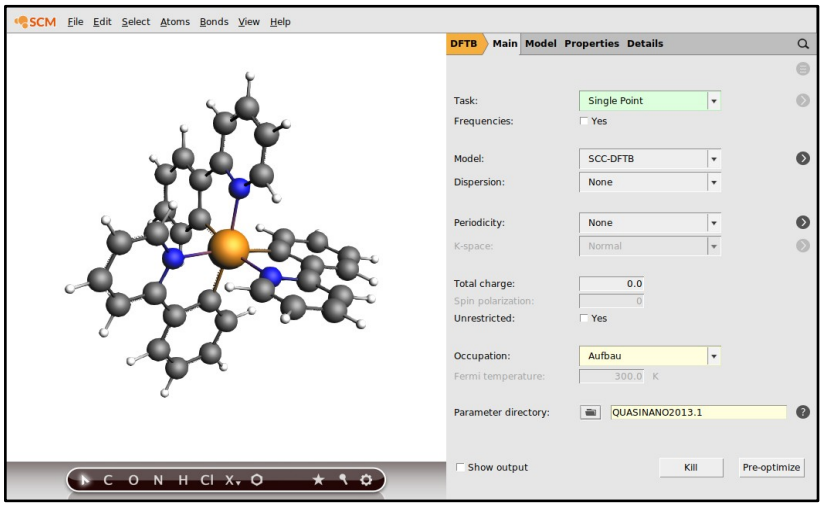
- Chained calculations
  - **Model Coordinates → Use: Job Result**
  - E.g. from prior (pre-) Optimization



- Presets: repeatedly access the same settings e.g. basis, functional, grid…
  - Select settings
  - **File → Save as preset** (difference from default)
  - **File → Save as full preset** (all input options)
  - Load via: **File → Preset → <PresetName>**
- AMSprepare & (report)
  - In AMSjob: select job, **tools → prepare**
  - AMSreport to gather & visualize results

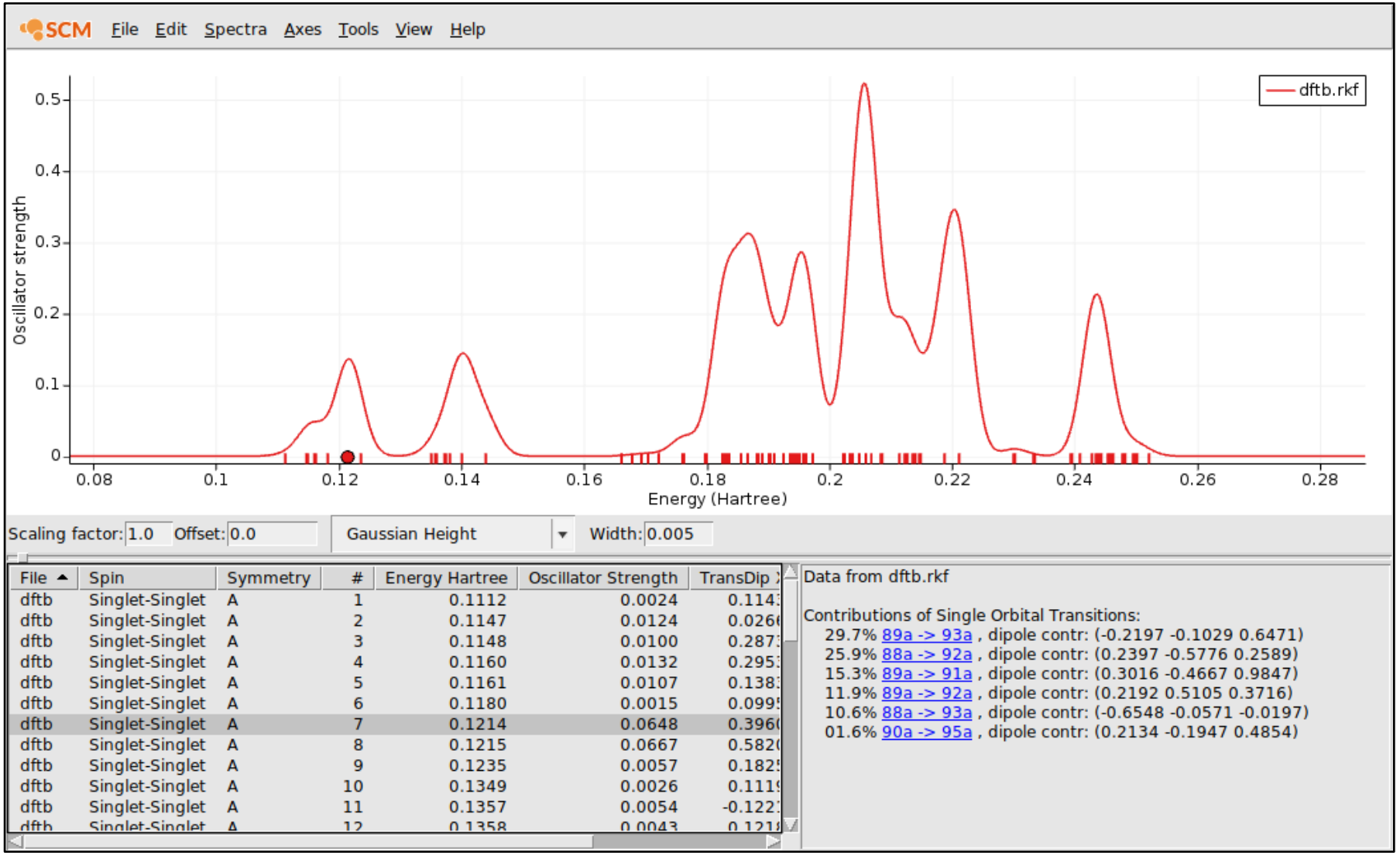
UV/Vis spectrum of $Ir(ppy)_3$

- **SCM → New Input**
- **ADF → DFTB**
  - **Task → Single Point**
  - **Model → SCC-DFTB**
  - **Occupation → Aufbau**
  - **Parameter directory → QUASINANO2013.1**
- TDDFTB-Settings: **Properties → Excitations (UV/VIS)**
  - **Type of excitations: → Singlet**
  - **Number of excitations: → 1000**
  - **Excitations up to: → 0.25 Hartree**
- Save and Run calculation



UV/Vis spectrum of $Ir(ppy)_3$

- **SCM → Spectra**



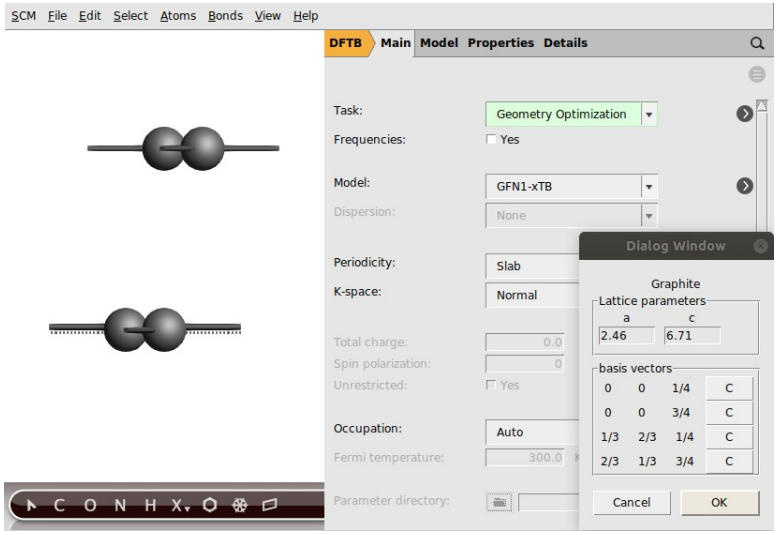
Periodic Structures

- 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
```

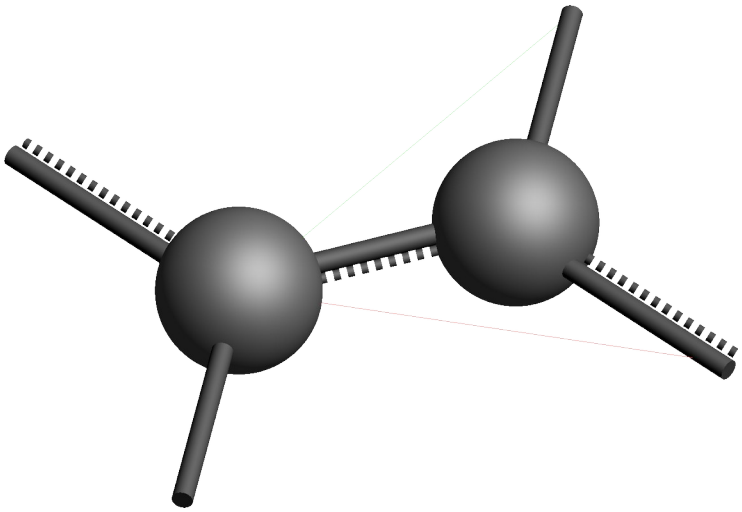
- Common structures from library
  - Switch to periodic engine e.g. ADF → DFTB
  - Periodicity → Bulk
  - Crystal structure library:
    
    → Hexagonal → Graphite



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



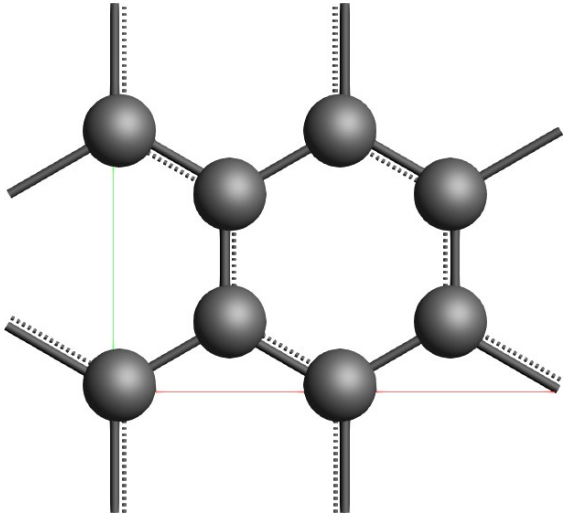
Tip: **Edit → Crystal**
→ Map Atoms to (0 .. 1)

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

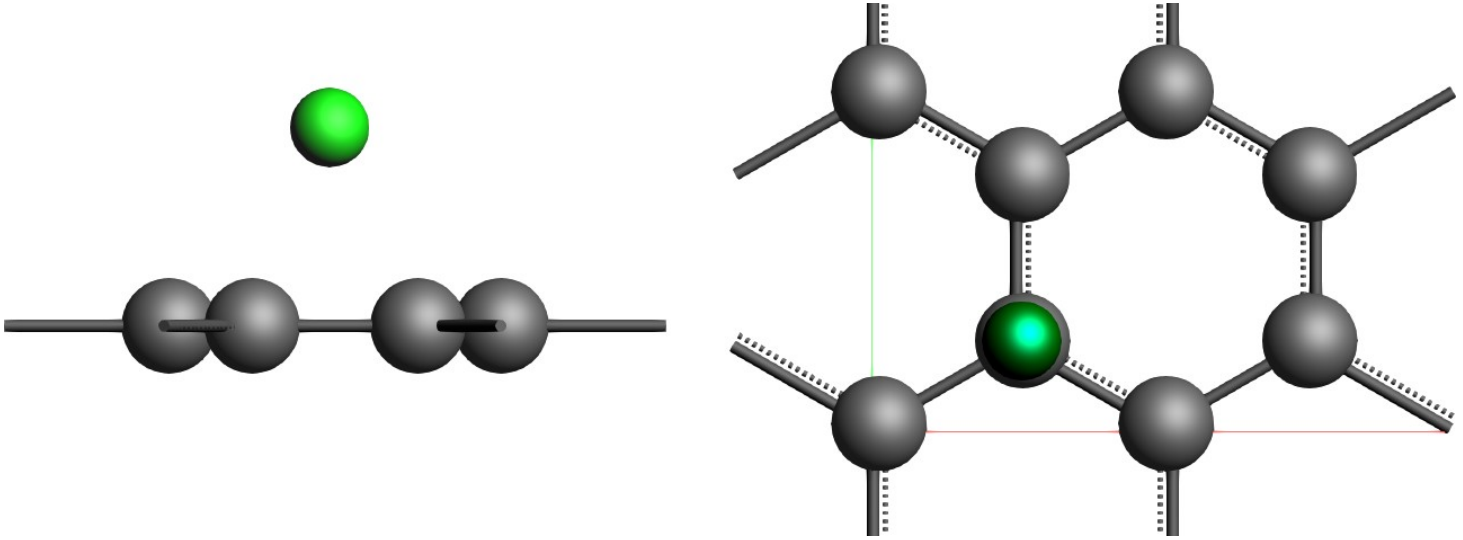
- Adsorption needs a bigger unit cell
  - Edit → Crystal → Generate Super Cell..
  - Enter coefficients 2 0 and -1 2 in popup mask for rectangular cell



- Export Coordinates → .xyz and save for later

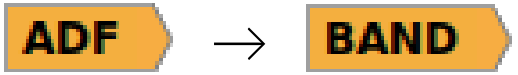
Adsorption Complex

- 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

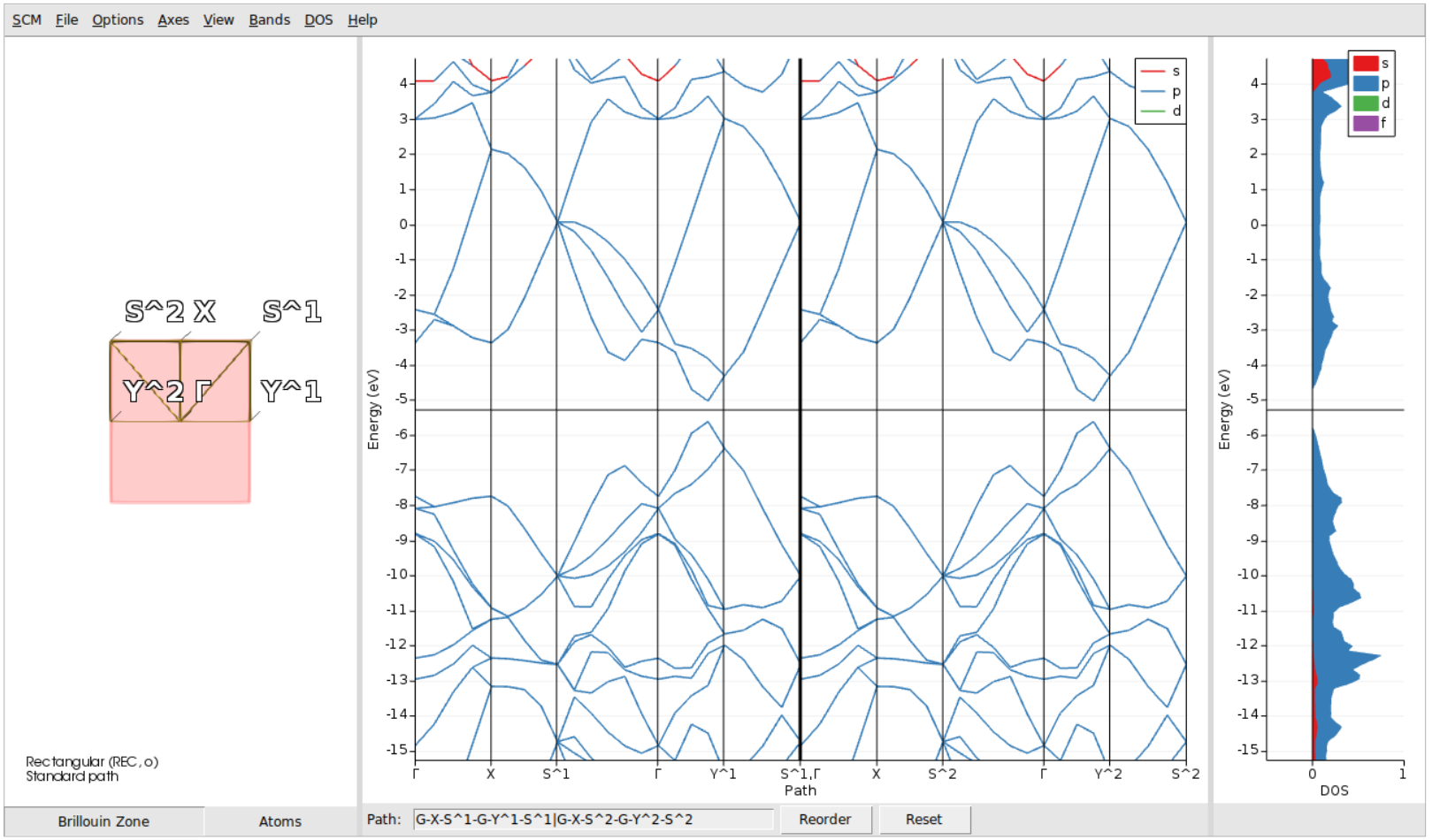
DFT Calculations for DOS & Band Structure

- 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

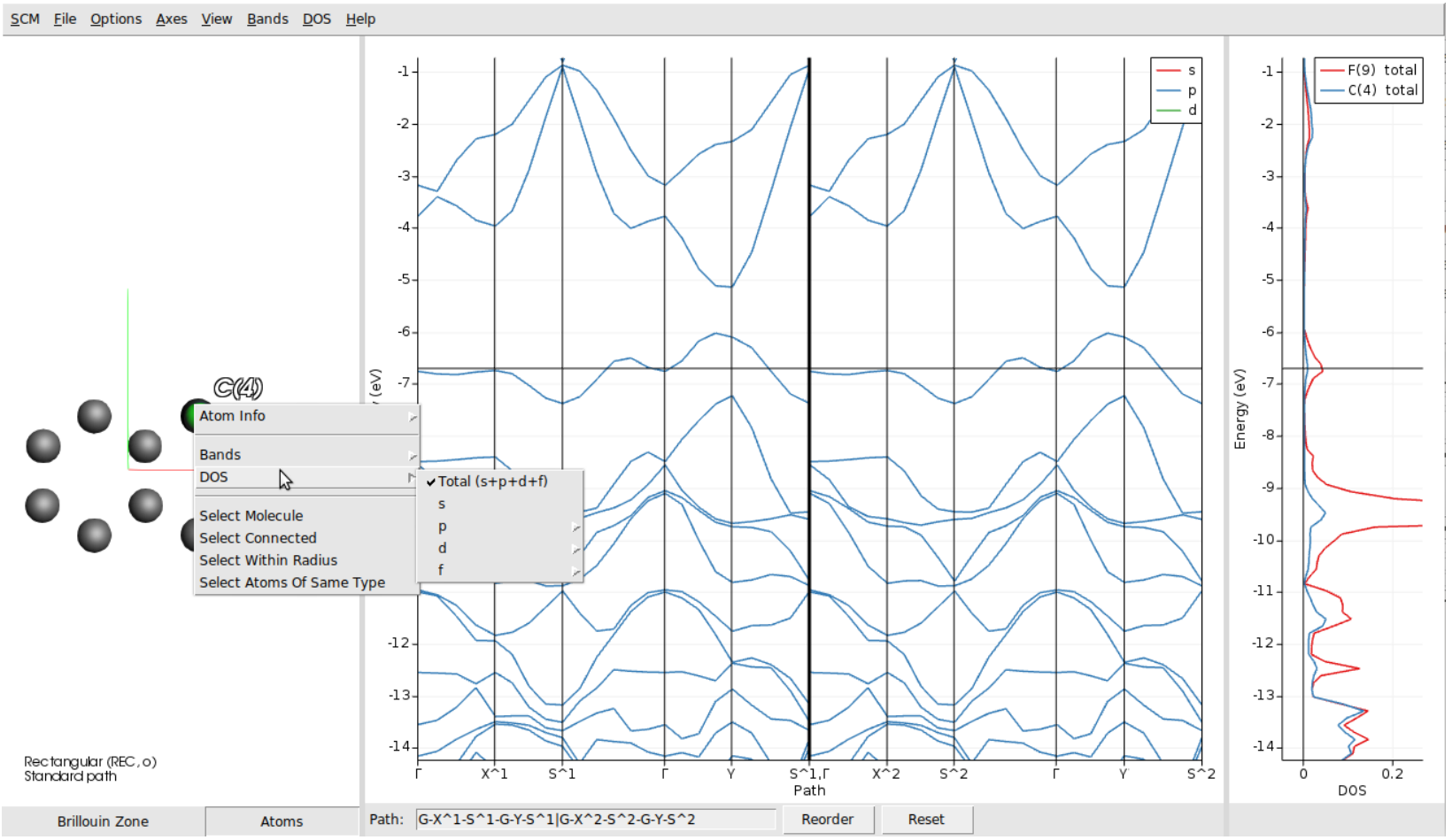
DOS & Band Structure

- 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

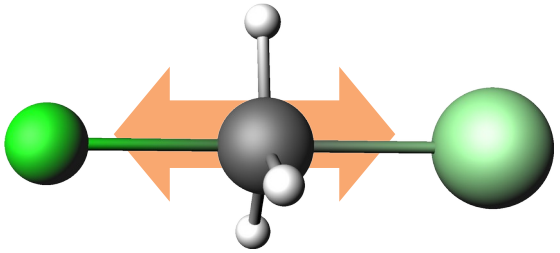


Transition States

- Transition state search for stationary point along reaction coordinate needed for reaction mechanism, barrier heights, reaction rates
- Two main approaches available in AMS
  - Quasi-Newton: needs estimate for TS structure and (usually) definition of the reaction mode
  - Nudged Elastic Band (NEB): samples entire reaction path

Molecular SN_2 Reaction

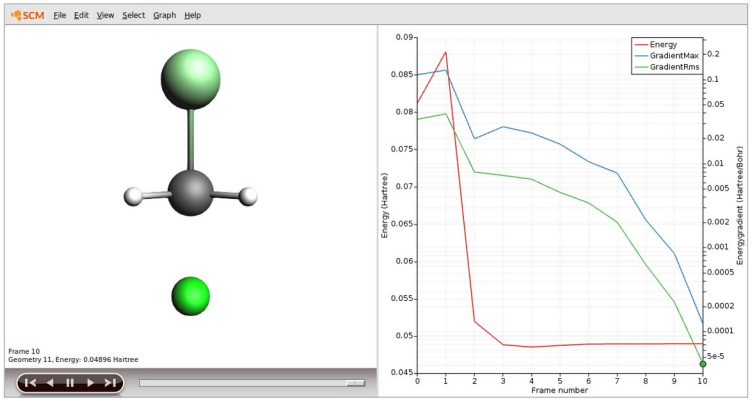
- In AMSinput: build Cl···CH_3···F guess (or import ClCH3F.xyz)



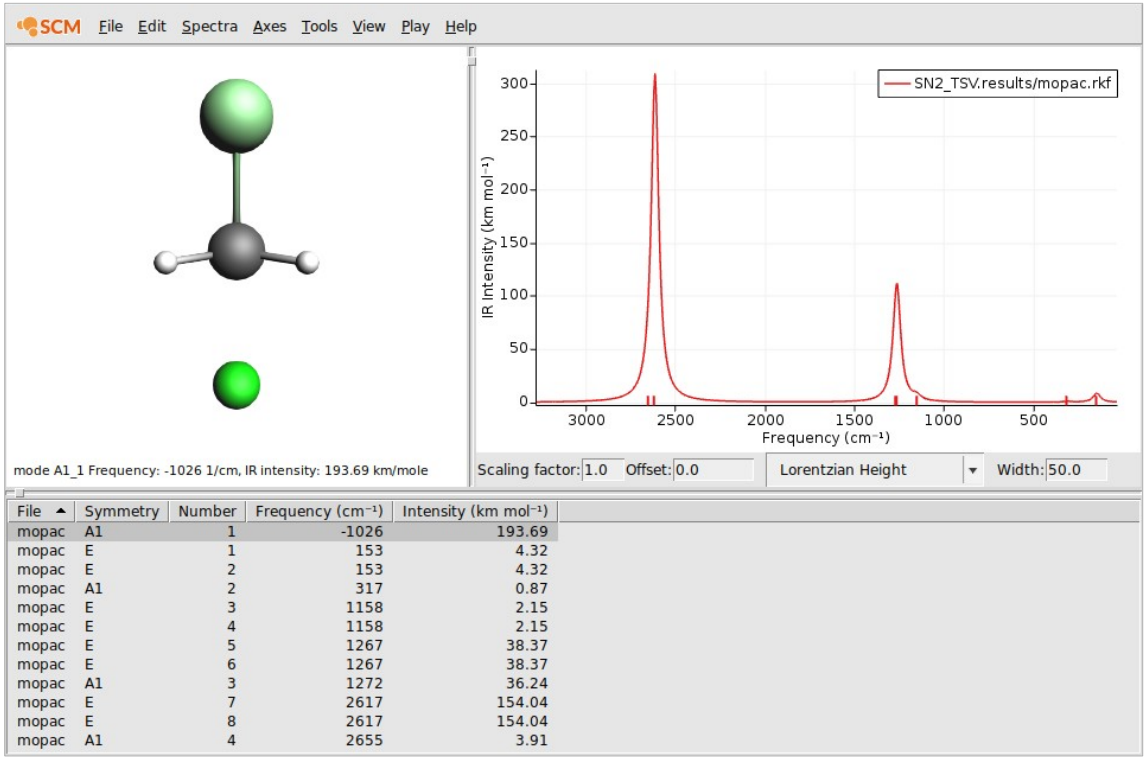
- Switch **ADF** → **Mopac**
  - **`Task` → `Transition State`**
    for larger systems ❯ to set details e.g. reaction coordinate
  - **`Frequencies`** → tick ☐ **`Yes`**
  - **`Spin polarization` → `1`**
- Save and run job

SN2 Transition State Analysis

- **`SCM → Movie`**
  to inspect transition state search



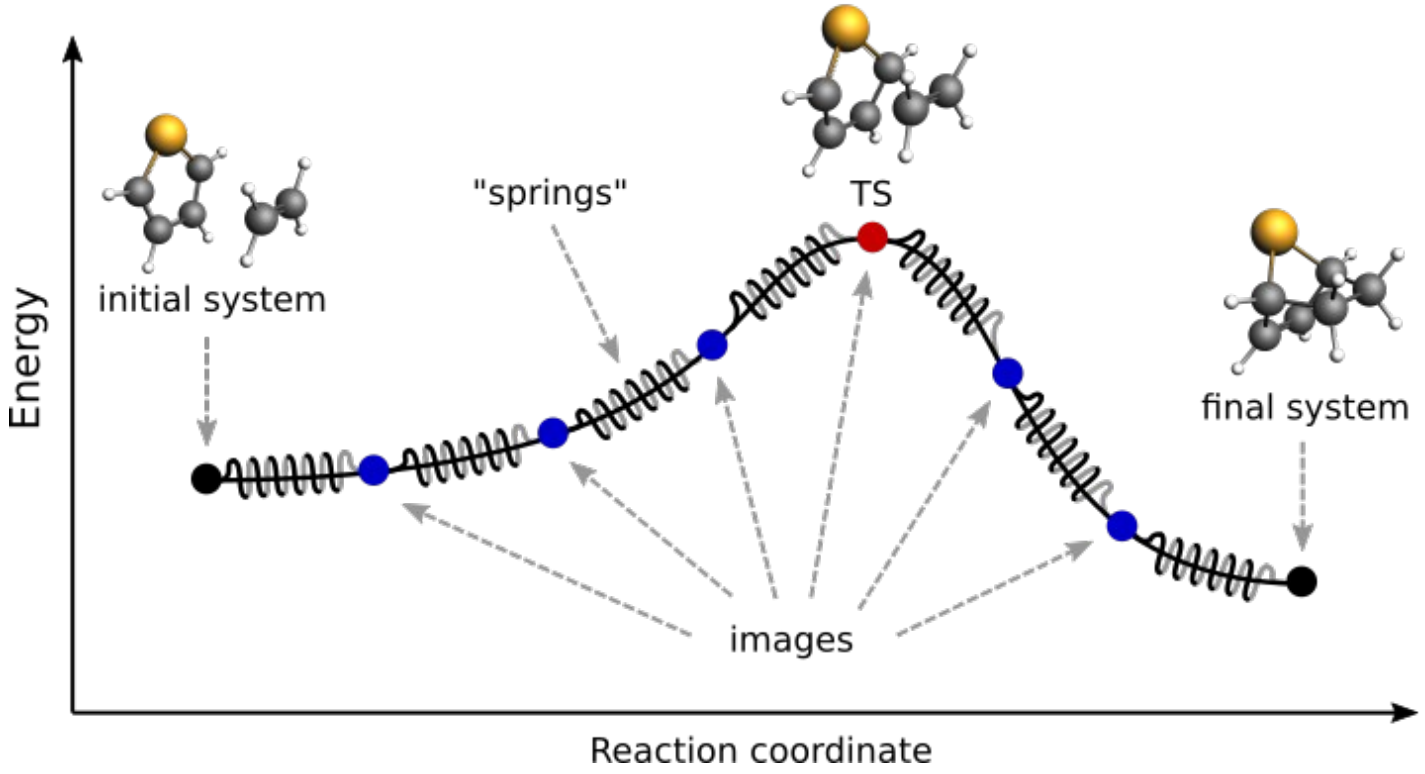
- **`SCM → Spectra`**
  to analyze reaction mode
  - *One* negative frequency
  - Click on negative mode to see movie of motion



File	Symmetry	Number	Frequency (cm⁻¹)	Intensity (km mol⁻¹)
mopac	A1	1	-1026	193.69
mopac	E	1	153	4.32
mopac	E	2	153	4.32
mopac	A1	2	317	0.87
mopac	E	3	1158	2.15
mopac	E	4	1158	2.15
mopac	E	5	1267	38.37
mopac	E	6	1267	38.37
mopac	A1	3	1272	36.24
mopac	E	7	2617	154.04
mopac	E	8	2617	154.04
mopac	A1	4	2655	3.91

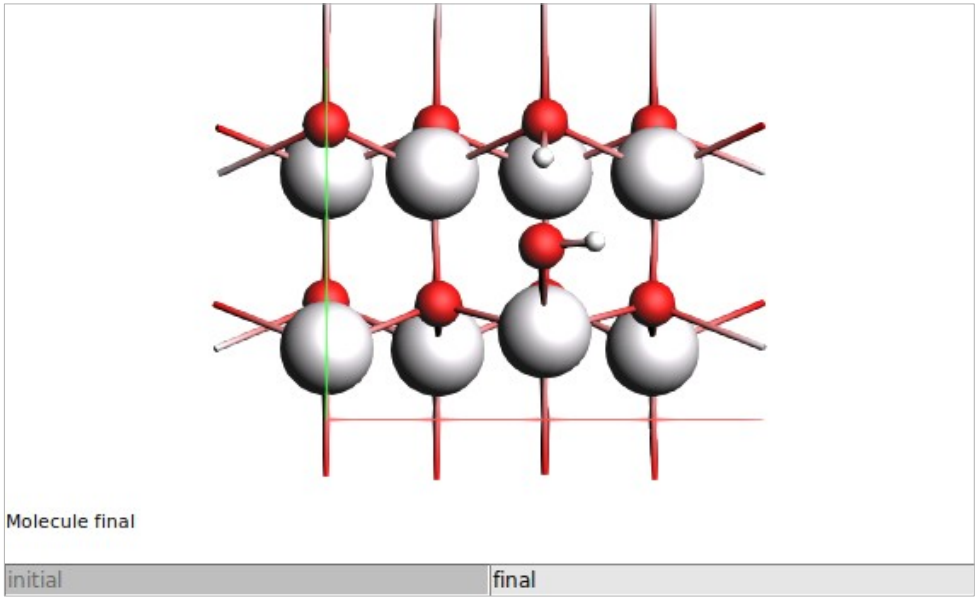
Nudged Elastic Band (NEB)

- Sample reaction path with multiple images (beads) of the system
- Adjacent images connected by “spring”
- Only coordinates orthogonal to the reaction path optimized



Surface Water Splitting Reaction with NEB

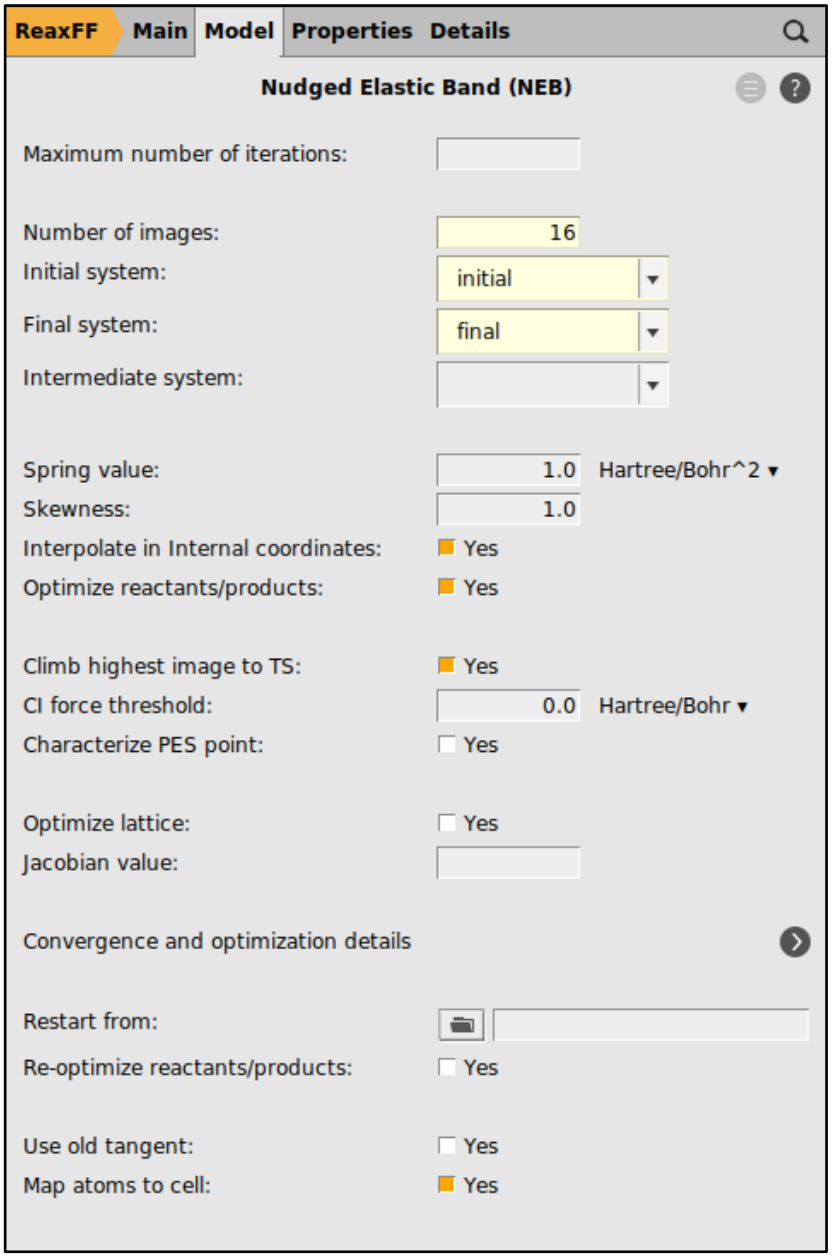
- AMSinput: import ZnOwatersplit_initial.xyz
- **`Edit` → `New Molecule`** opens new editor tab
- Switch to Mol-2 tab and import ZnOwatersplit_final.xyz



Tip: rename tabs to *initial* and *final* by double-clicking on them

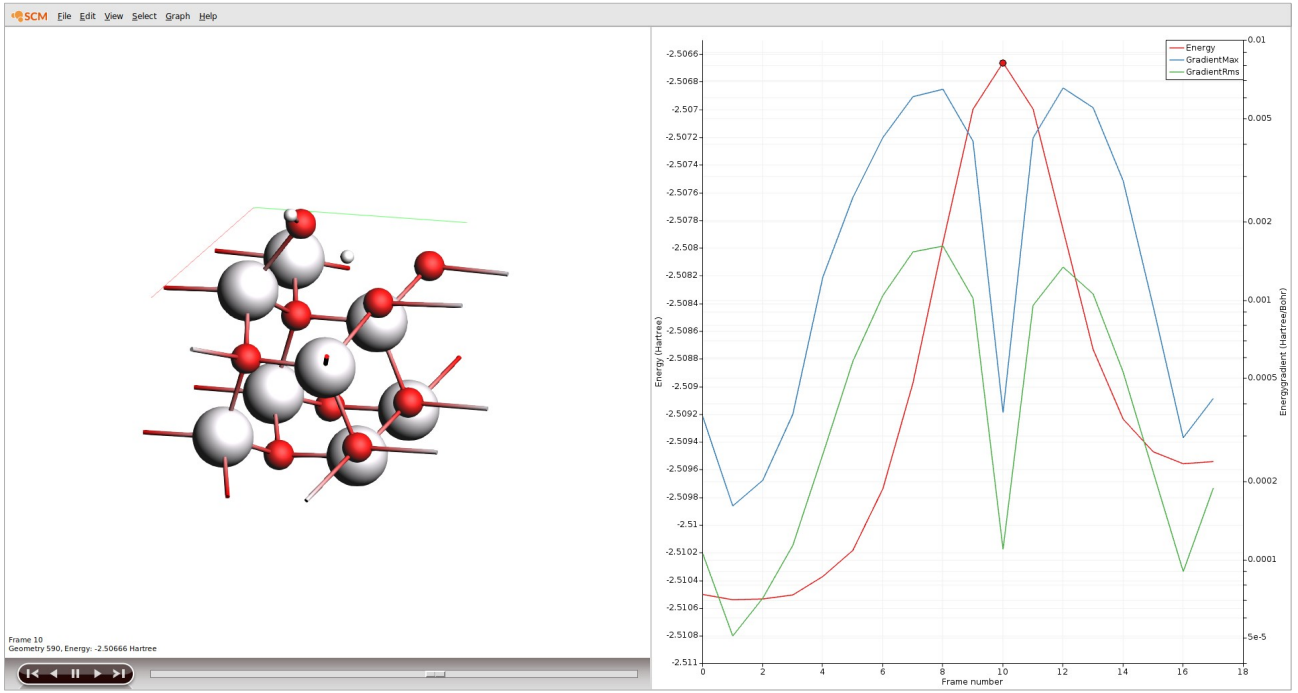
NEB Calculation

- Switch **BAND** → **ReaxFF**
- **Task** → **NEB** then click ❯ next to it
  - **Number of images** → **16**
  - **Initial system** → *Mol-1* (or *initial*)
    Final system → *Mol-2* (or *final*)
- Return to **Main** panel
  - **Frequencies** → tick ☐ **Yes**
  - **Force Field** → **ZnOH.ff**
- Save and run calculation



NEB Reaction Path

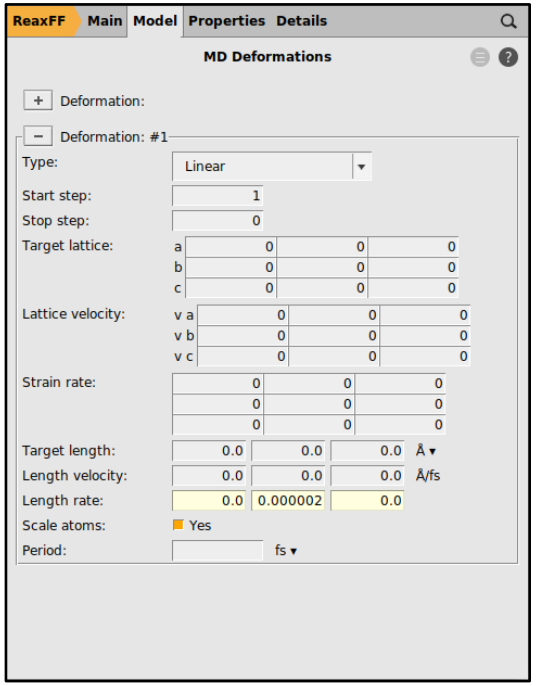
- **SCM** → **Movie** to examine NEB path



- **SCM** → **Spectra** to confirm the correct reaction mode

Snapping Polymer Chain

- **File → Import Coordinates → cis_polyacetylene.xyz**
- **BAND → ReaxFF**
  - **Force Field → CHO.ff**
- **Task: → Molecular Dynamics**, then click
  - **Number of steps: → 80000**
- **Thermostat:** click
  - **Thermostat: → NHC**
  - **Temperature: → 300.15**
  - **Damping constant: → 100 fs**
- **Model → MD deformations**
  - **Length rate →** Y: **0.000002**
- **Properties → Gradients, Stress tensor**
  - **Stress tensor →** tick ☐ **Yes**



Snapping Polymer Chain

- Save and run calculation
- **SCM → Movie** to monitor progress
- Switch to console
  - Linux/Mac OSX: **`source amsbashrc.sh`**
  - Windows: start **`ams_command_line.bat`**
  - **`amspython stress_strain_curve.py <JobName>`**
  - **`amspython plot_stress.py stress-strain-curve.csv`**
- cis- and trans-configurations have different mechanical properties

Optional Exercise: Bouncing Buckyball

- https://www.scm.com/doc/Tutorials/moleculardynamicsandmontecarlo/moleculegun.html