

Amsterdam Modeling Suite



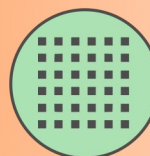
AMS
driver



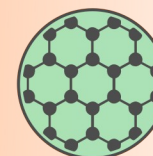
GUI



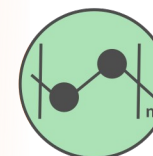
PLAMS



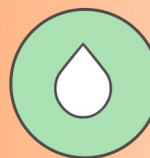
Organic
Electronics



Materials



Polymers



Oil & Gas



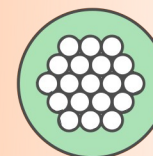
Batteries



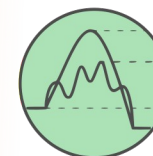
Pharma



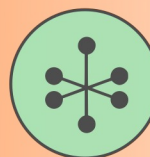
Spectroscopy



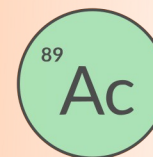
Nanoscience



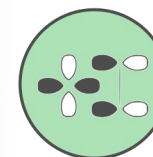
Catalysis



Inorganic
Chemistry



Heavy
Elements

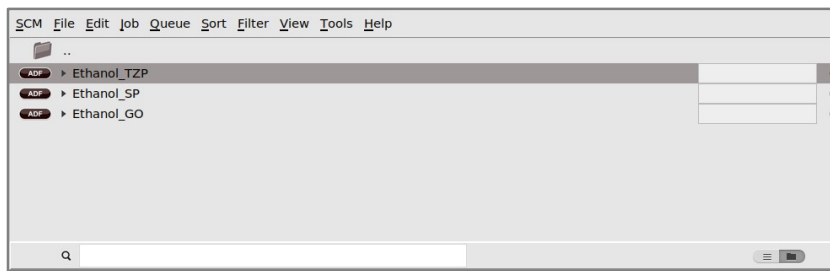


Bonding
Analysis

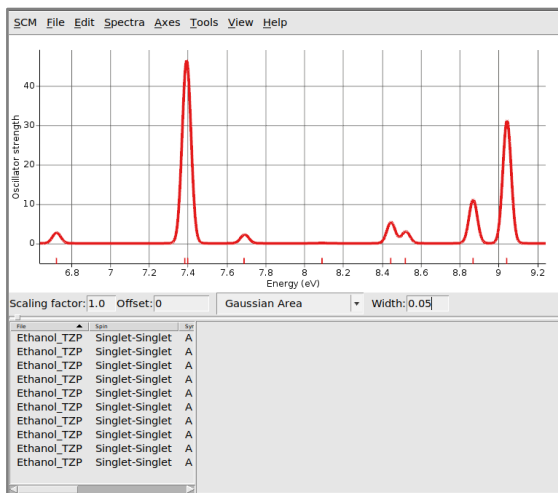
GUI Modules



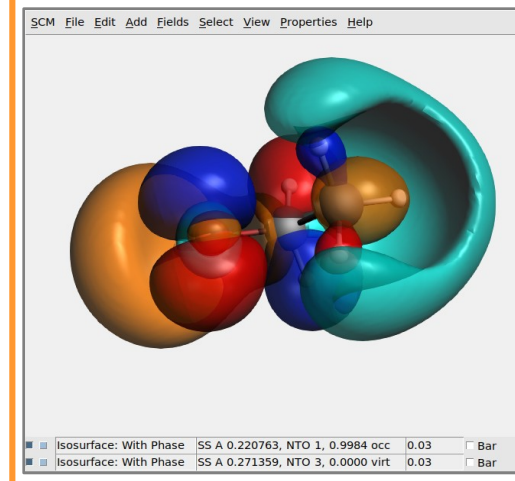
AMSjobs – Calculation Management



AMSspectra – Spectra



AMSview – 3D Plots



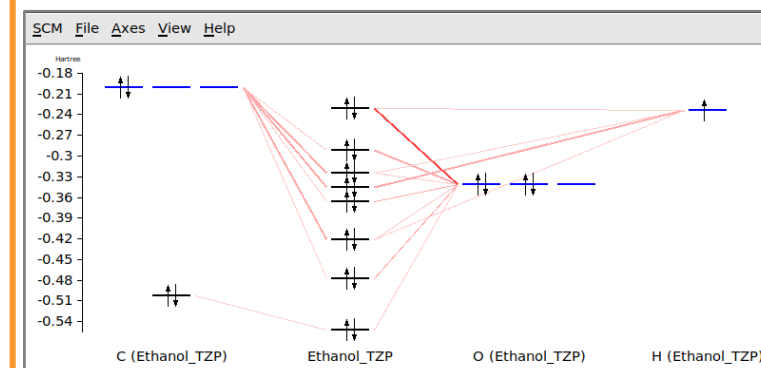
AMSinput – Editor & Settings

Task: Single Point
Frequencies: Yes
Total charge: 0.0
Spin polarization: 0.0
Unrestricted: Yes
XC functional: LDA
Relativity: Scalar
Basis set: DZ
Froze core: Large
Numerical quality: Normal

AMSoutput – Text Results

```
*****  
* Amsterdam Modeling Suite (AMS) 2020.203 *  
* r91208 2021-01-27 *  
*  
* A M S *  
*****
```

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>**

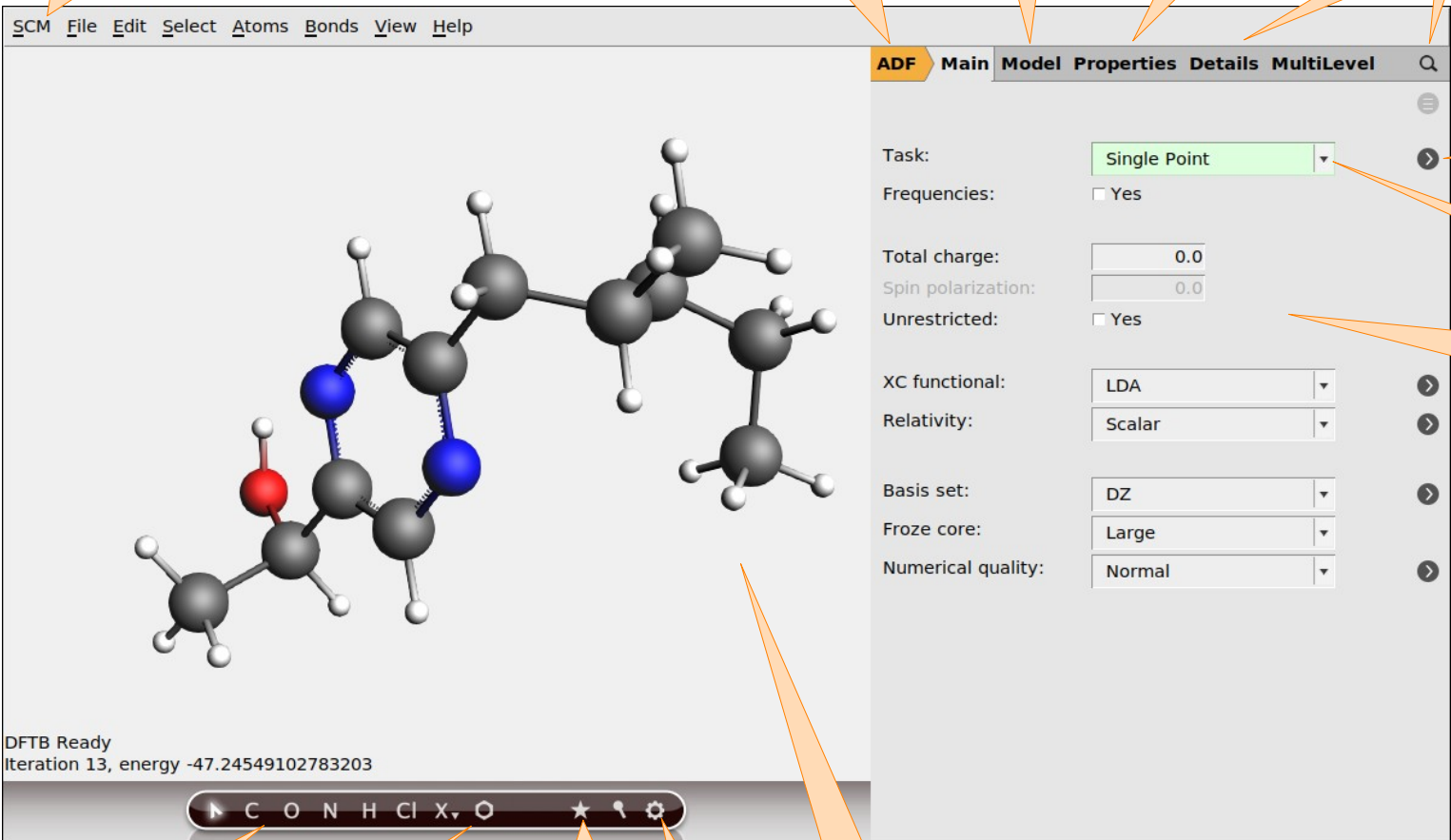
AMSjobs



The screenshot shows the AMSjobs application interface with several callout boxes:

- SCM-button: switch module**: Points to the 'SCM' menu item in the top bar.
- Job controls**: Points to the 'Job' menu item.
- Batch jobs, reports, templates**: Points to the 'Queue' menu item.
- Queue selection & setup**: Points to the 'Queue' menu item.
- Options: cores, nodes, walltime**: Points to the 'Sort' menu item.
- Queue**: Points to the 'sky' queue name in the job list.
- See input & output files**: Points to the 'Ethanol_SP' job entry.
- Job type**: Points to the 'ADF' button next to the job entries.
- Search**: Points to the search bar at the bottom left.
- View folders / all jobs**: Points to the folder icons in the top left.
- Job status**: Points to the status icons (red, black, white circles) on the right side of the job list.

Job Name	Queue	Options	Status
Ethanol_GO	sky	1	Red circle
Ethanol_TZP	Sequential		Black circle
Ethanol_SP			White circle



The screenshot shows the AMSinput software interface. The main window displays a ball-and-stick model of a complex organic molecule. The interface includes a menu bar at the top with options: SCM, File, Edit, Select, Atoms, Bonds, View, Help. Below the menu bar is a tabbed interface with tabs: ADF, Main, Model, Properties, Details, MultiLevel. The right side of the interface contains a settings panel with various options and values:

- Task: Single Point
- Frequencies: Yes
- Total charge: 0.0
- Spin polarization: 0.0
- Unrestricted: Yes
- XC functional: LDA
- Relativity: Scalar
- Basis set: DZ
- Froze core: Large
- Numerical quality: Normal

At the bottom of the interface is a toolbar with icons for navigation and editing. The callout boxes identify the following features:

- SCM-button: switch module
- System & Task details
- Search library & manual
- Switch engine
- Results
- Technical settings
- Details
- Task
- Settings panels
- Elements
- Template Structures
- Symmetrize
- Preoptimize
- Molecular editor

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

The screenshot displays the SCM Molecular Editor interface. At the top, a menu bar includes 'SCM', 'File', 'Edit', 'Select', 'Atoms', 'Bonds', 'View', and 'Help'. Below the menu, a toolbar contains icons for navigation and atom selection, with 'C' and 'O' highlighted. A 3D ball-and-stick model of a molecule is shown in the center, with a mouse cursor pointing at one of the atoms. Below the model, the text 'C(2), 4 connectors' is visible. To the right of the model, the labels 'C-tool' and 'O-tool' are present, with orange arrows pointing to the 'C' and 'O' buttons in the toolbar. A tooltip for the 'O' button reads 'O tool, create single bond'. On the right side of the interface, a properties panel is open, showing various computational parameters:

Property	Value
Task	Single Point
Total charge	0
Spin polarization	0
Unrestricted	<input type="checkbox"/> Yes
XC functional	LDA
Relativity (ZORA)	None
Basis set	DZ
Frozen core	Large
Numerical quality	Normal

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

The screenshot displays the SCM Molecular Editor interface. The main window shows a ball-and-stick model of a molecule with a highlighted hydroxyl (OH) group. A rectangular selection box is drawn around the OH group, and a mouse cursor is positioned at the bottom-right corner of this box. Below the model, the word "preoptimizer" is written in a bold, black, sans-serif font. An orange arrow points from this text to a gear icon in the bottom toolbar. The right-hand side of the interface features a panel with various computational settings, including a task dropdown set to "Single Point", total charge and spin polarization set to 0, and various functional and basis set options.

SCM File Edit Select Atoms Bonds View Help

ADF Main Model Properties Details MultiLevel

Task: Single Point

Total charge: 0

Spin polarization: 0

Unrestricted: Yes

XC functional: LDA

Relativity (ZORA): None

Basis set: DZ

Frozen core: Large

Numerical quality: Normal

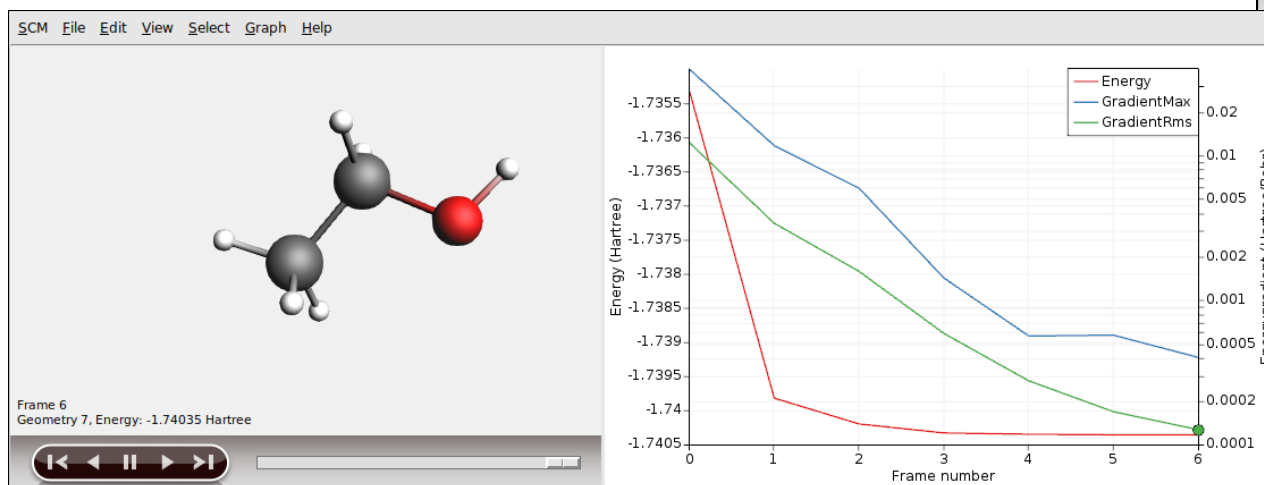
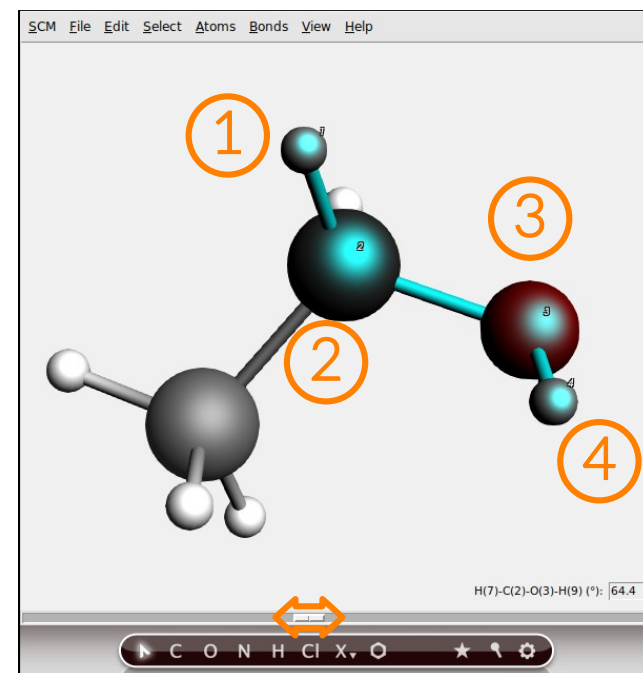
preoptimizer

C O N H Cl X O ★ 🔍 ⚙️

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**

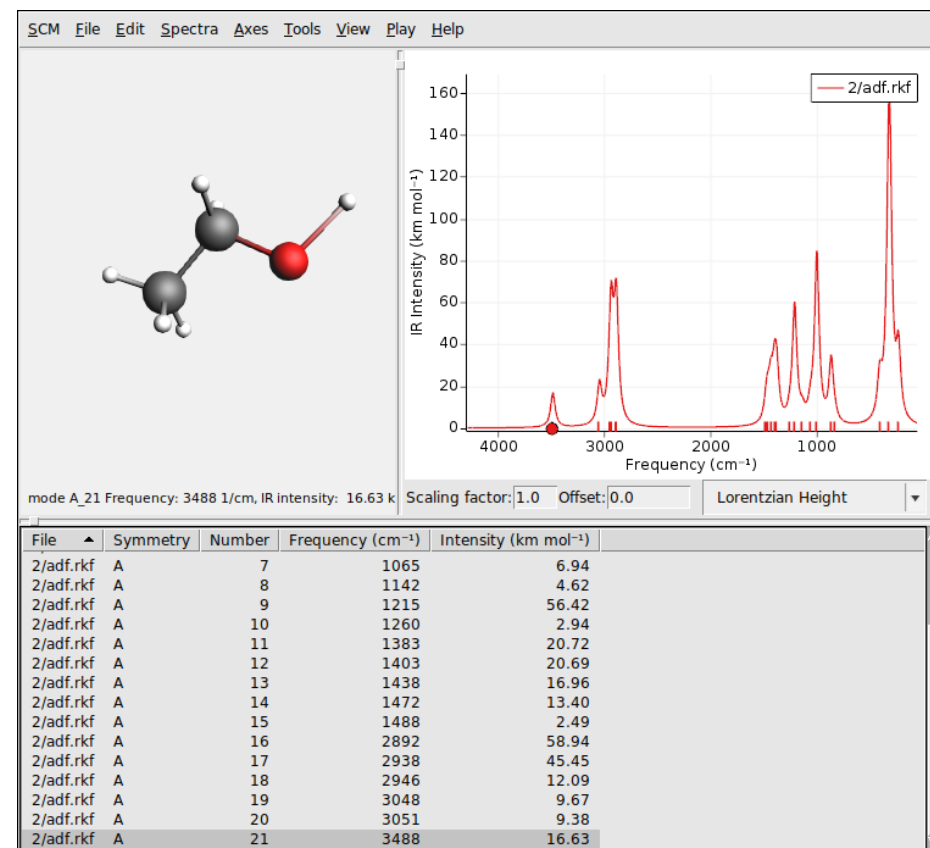


Load Results & Frequency Calculation



- ▶ **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

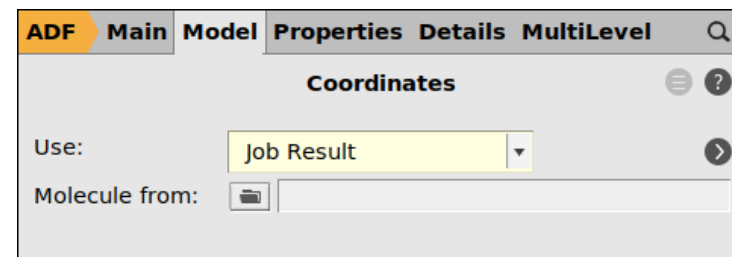
Tip: **ams.rkf** contains driver results (optimization, MD trajectory etc.)
<engine>.rkf contains engine-related data and results



GUI Efficiency Tricks & Features



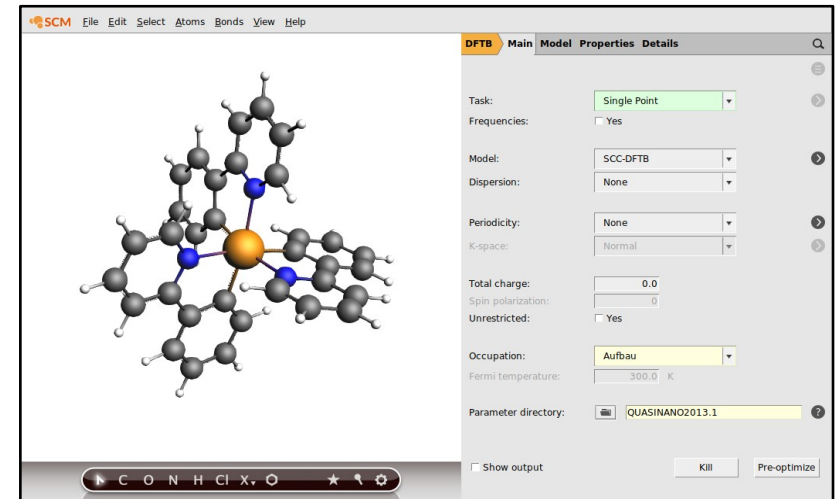
- ▶ Chained calculations
 - ▶ **Model Coordinates** → Use: Job Result
 - ▶ E.g. from prior (pre-) Optimization
- ▶ Presets: repeatedly access the same settings e.g. basis, functional, grid...
 - ▶ Select settings
 - ▶ **File** → **Save as preset** (difference from default)
 - ▶ **File** → **Save as full 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



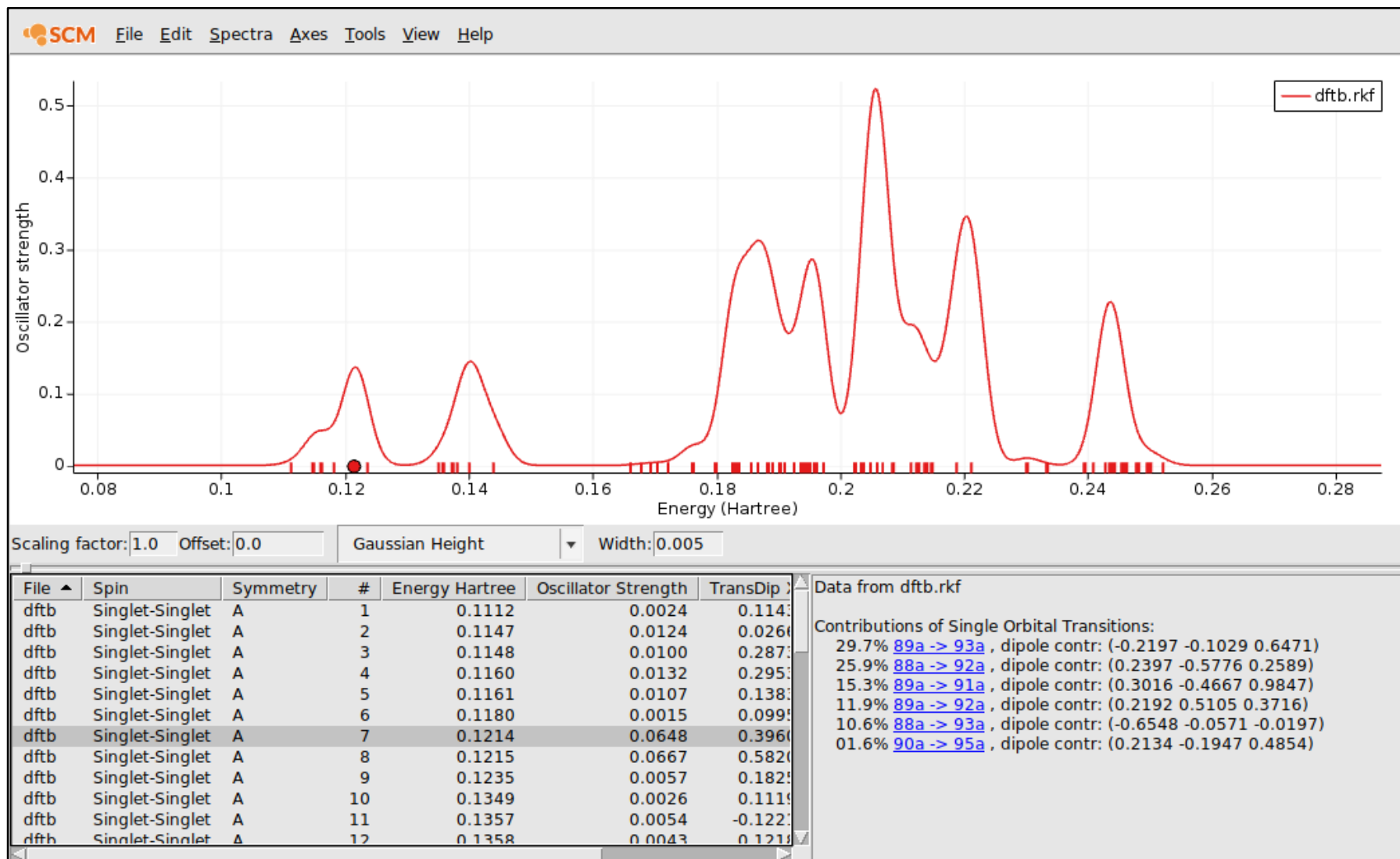
- ▶ **SCM → New Input**
- ▶ **ADF → DFTB**
 - ▶ **Task → Single Point**
 - ▶ **Model → SCC-DFTB**
 - ▶ **Occupation → Aufbau**
 - ▶ **Parameter directory → QUASINANO2013.1**
- ▶ **TDDFTB-Settings: Properties → Excitations (UV/VIS)**
 - ▶ **Type of excitations: → Singlet**
 - ▶ **Number of excitations: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



UV/Vis spectrum of Ir(ppy)₃



► SCM → Spectra



Periodic Structures

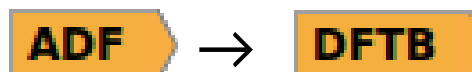
▶ File → Import Coordinates → cif/POSCAR/xyz

▶ 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.

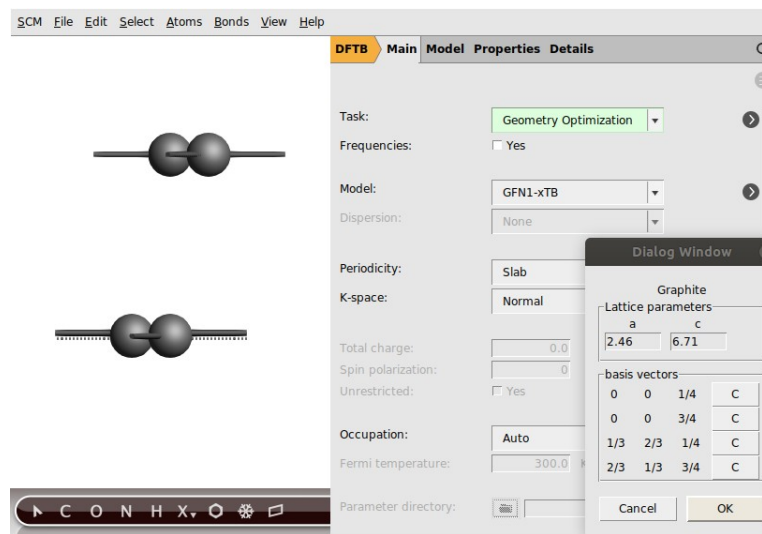


▶ Periodicity → Bulk

▶ Crystal structure library:



→ Hexagonal → Graphite



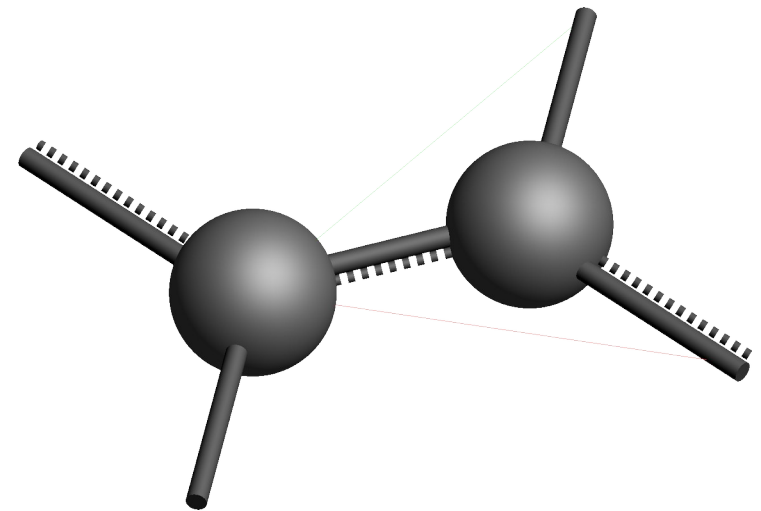
The screenshot shows the SCM software interface. The main window displays the DFTB engine settings, including Task: Geometry Optimization, Model: GFN1-xTB, and Periodicity: Slab. A dialog window titled "Dialog Window" is open, showing the Graphite lattice parameters: a = 2.46, c = 6.71, and the basis vectors table.

Graphite			
Lattice parameters			
a	c		
2.46	6.71		
basis vectors			
0	0	1/4	C
0	0	3/4	C
1/3	2/3	1/4	C
2/3	1/3	3/4	C

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)**

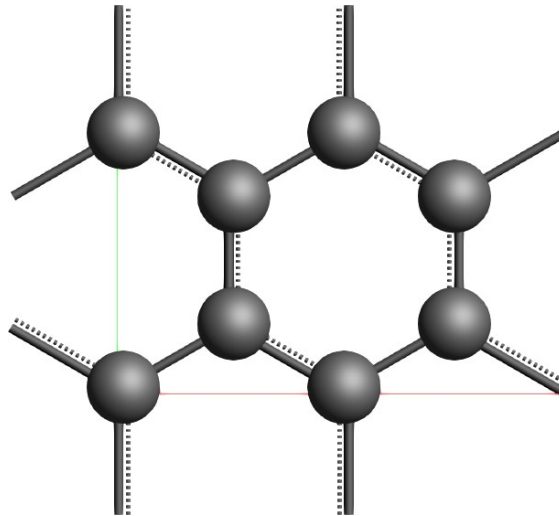
Lattice Optimization



- ▶ 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

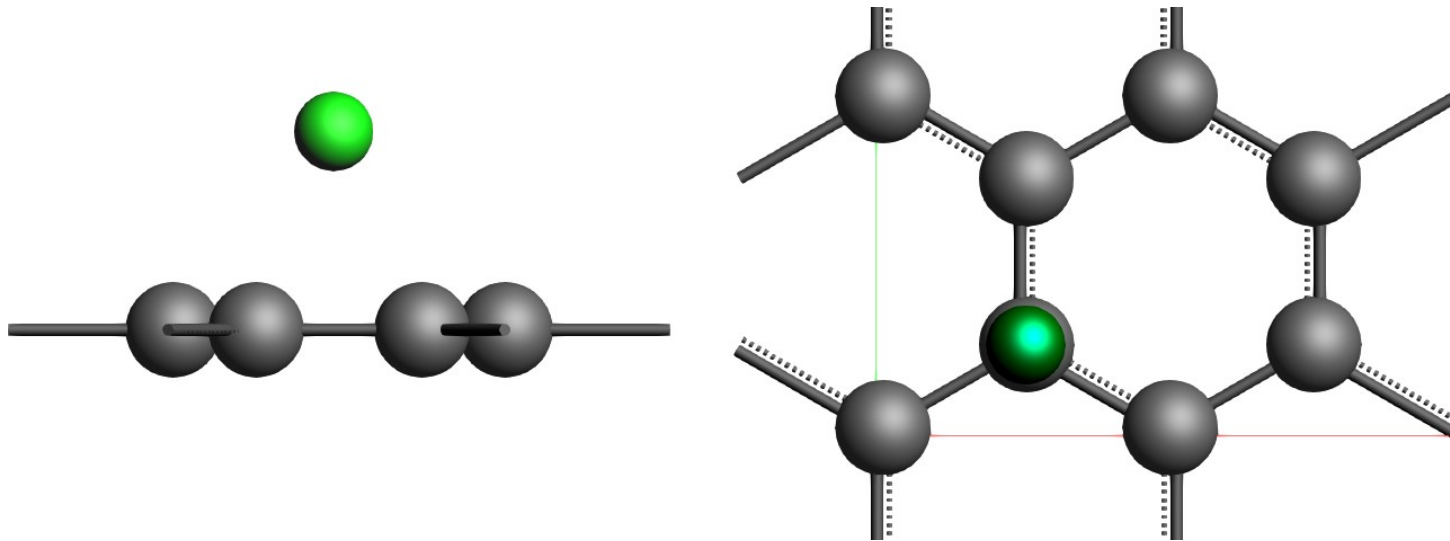
- ▶ Adsorption needs a bigger unit cell
 - ▶ Edit → Crystal → Generate Super Cell..
 - ▶ Enter coefficients $2\ 0$ and $-1\ 2$ in popup mask for rectangular cell




- ▶ 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

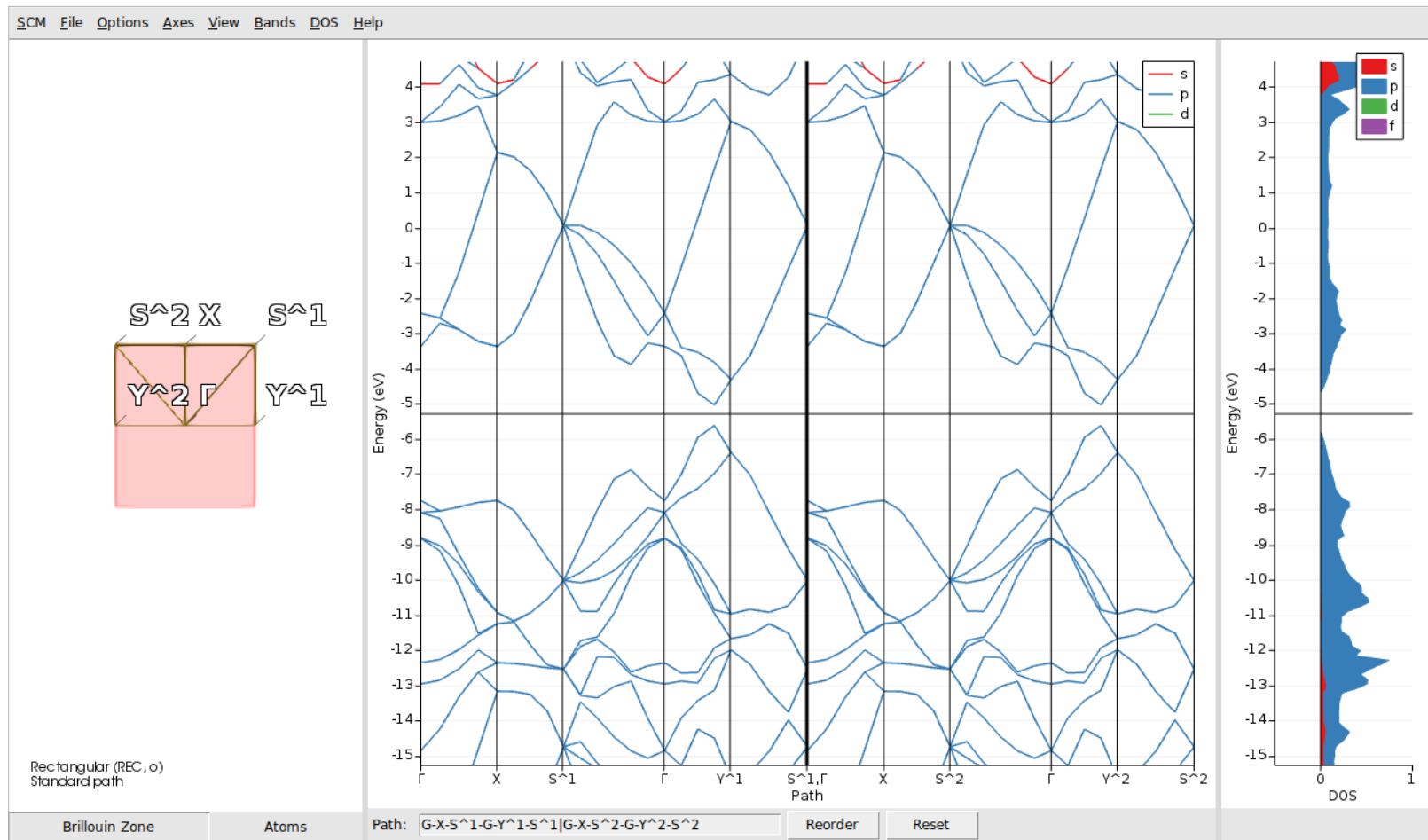


- ▶ Open new input
- ▶ File → Import Coordinates to load adsorption complex geometry
- ▶ Switch to BAND **ADF** → **BAND**
- ▶ Task → Single Point
- ▶ Calculate DOS → tick Yes
Calculate band structure → tick Yes
- ▶ Run calculation
- ▶ Repeat for Graphene Supercell structure

DOS & Band Structure



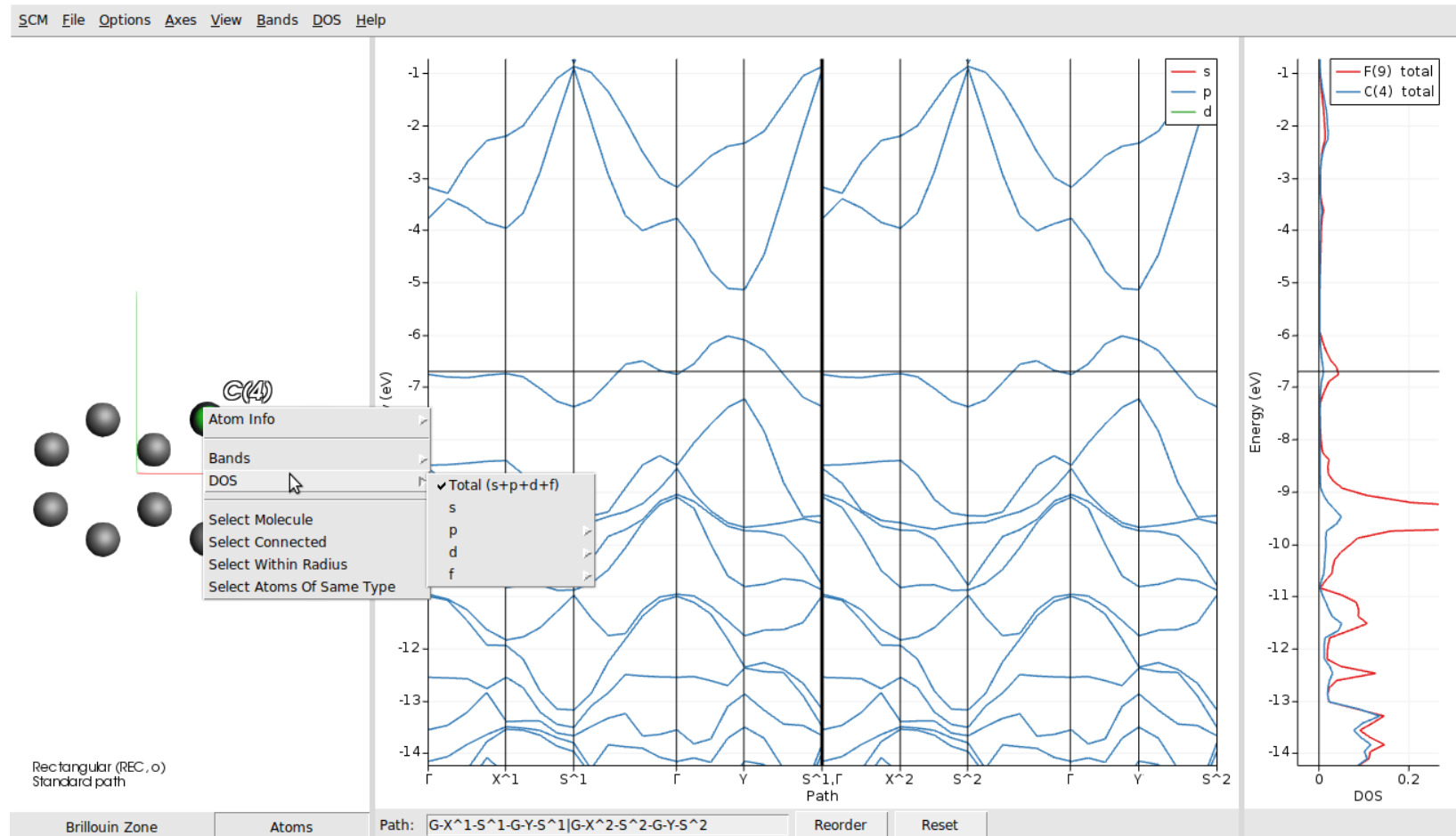
- ▶ SCM → band structure to visualize results



DOS & Band Structure



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



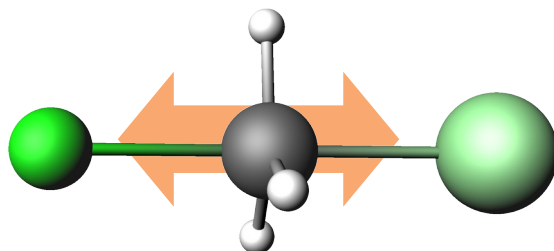
Transition States



- ▶ 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 $\text{S}_{\text{N}}2$ Reaction

- ▶ In AMSinput: build $\text{Cl}\cdots\text{CH}_3\cdots\text{F}$ guess (or import $\text{ClCH}_3\text{F.xyz}$)



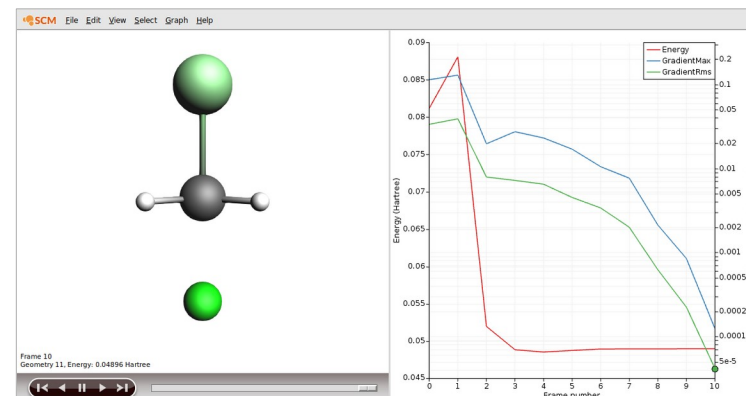
- ▶ Switch **ADF** → **Mopac**
 - ▶ **Task** → **Transition State**
for larger systems > to set details e.g. reaction coordinate
 - ▶ **Frequencies** → tick **Yes**
 - ▶ **Spin polarization** → **1**
- ▶ Save and run job

SN2 Transition State Analysis



▶ SCM → Movie

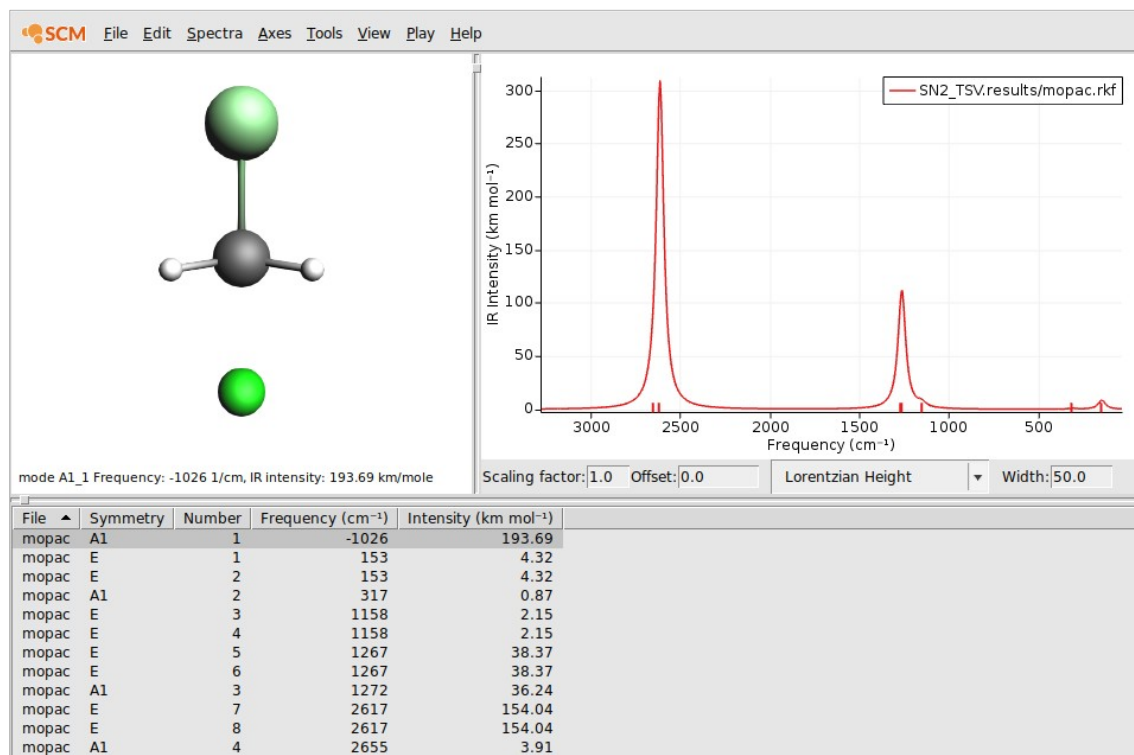
to inspect transition state search



▶ SCM → Spectra

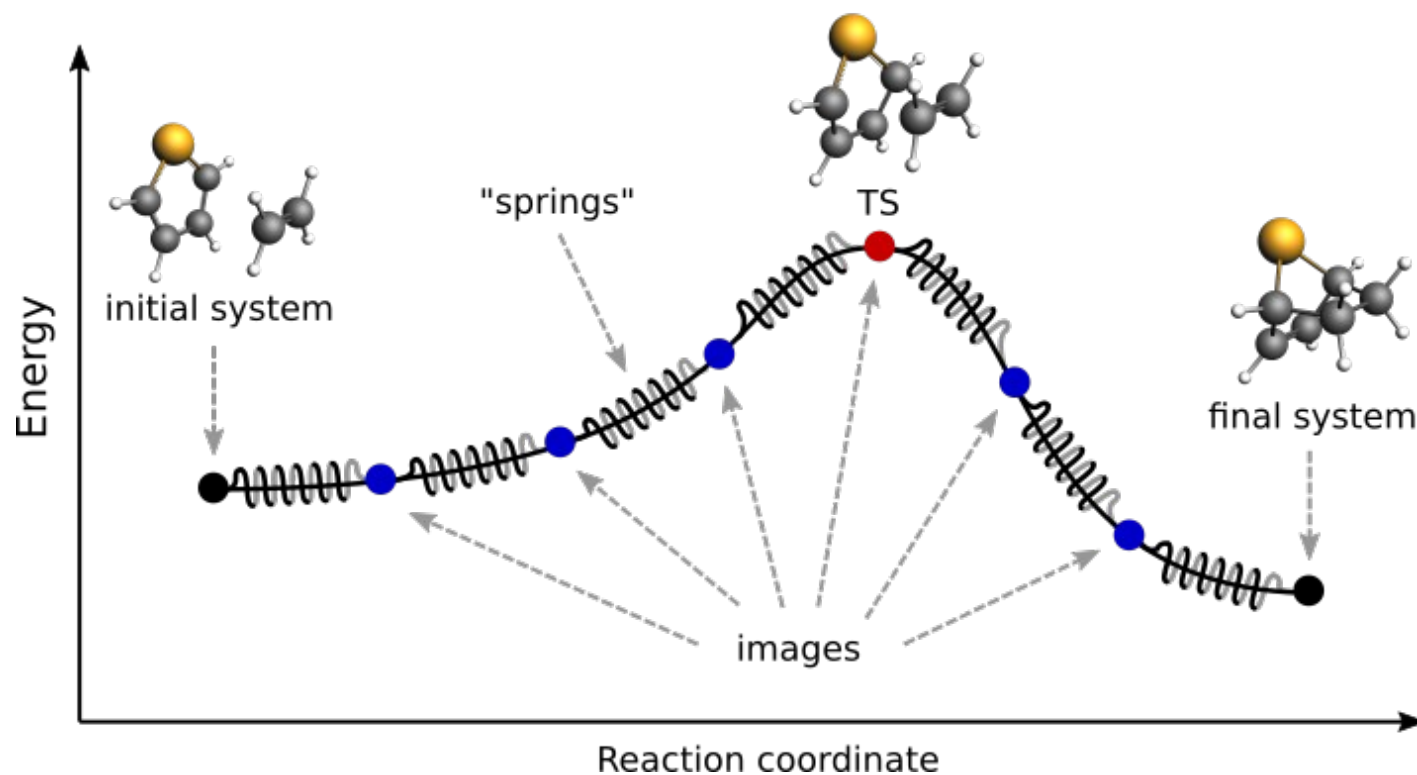
to analyze reaction mode

- ▶ One negative frequency
- ▶ Click on negative mode to see movie of motion



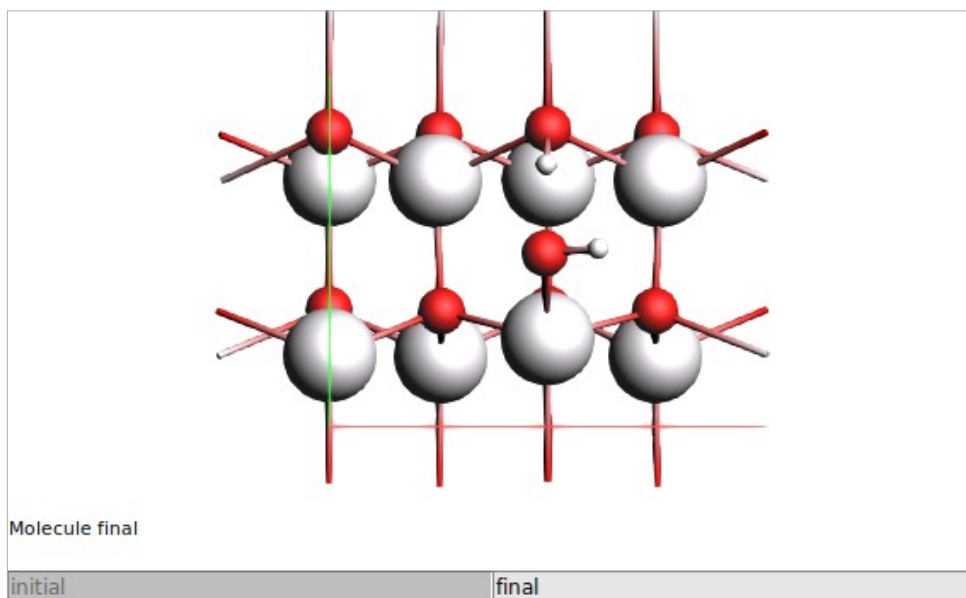
Nudged Elastic Band (NEB)

- ▶ 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

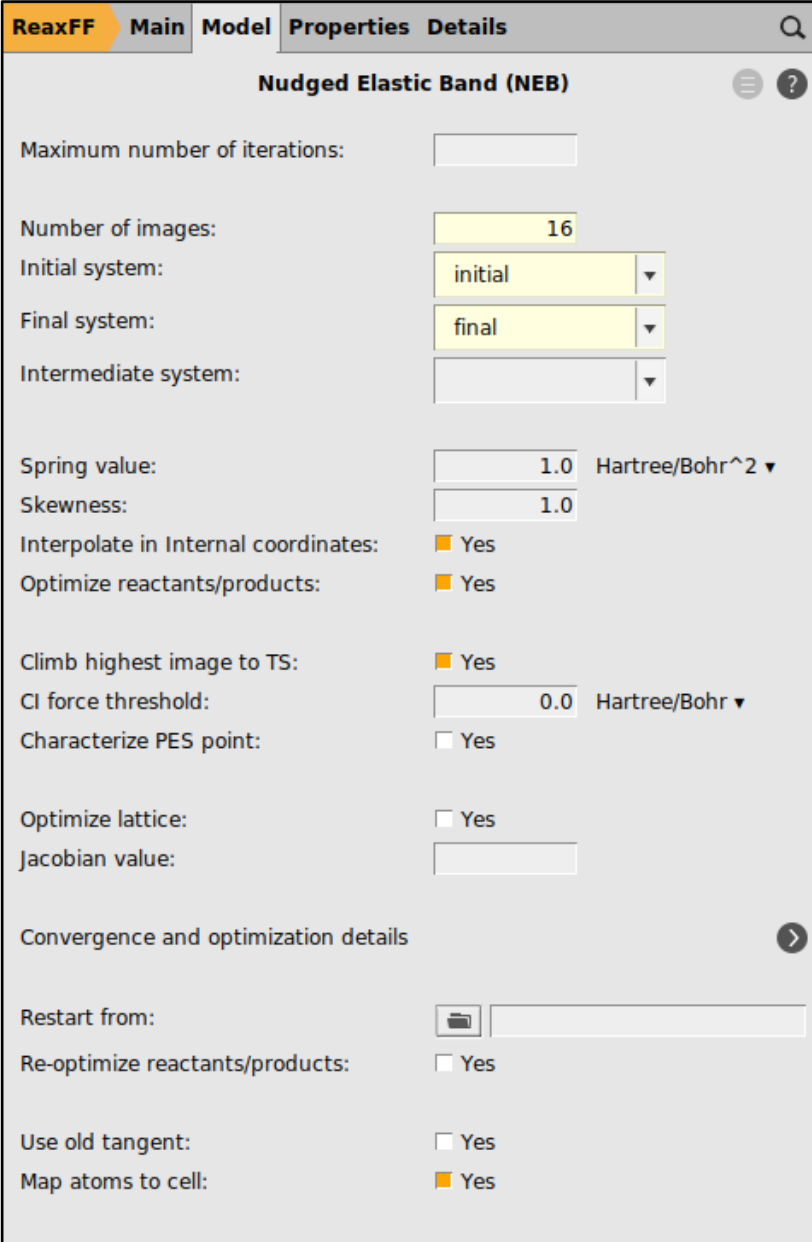


Tip: rename tabs to *initial* and *final* by double-clicking on them



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

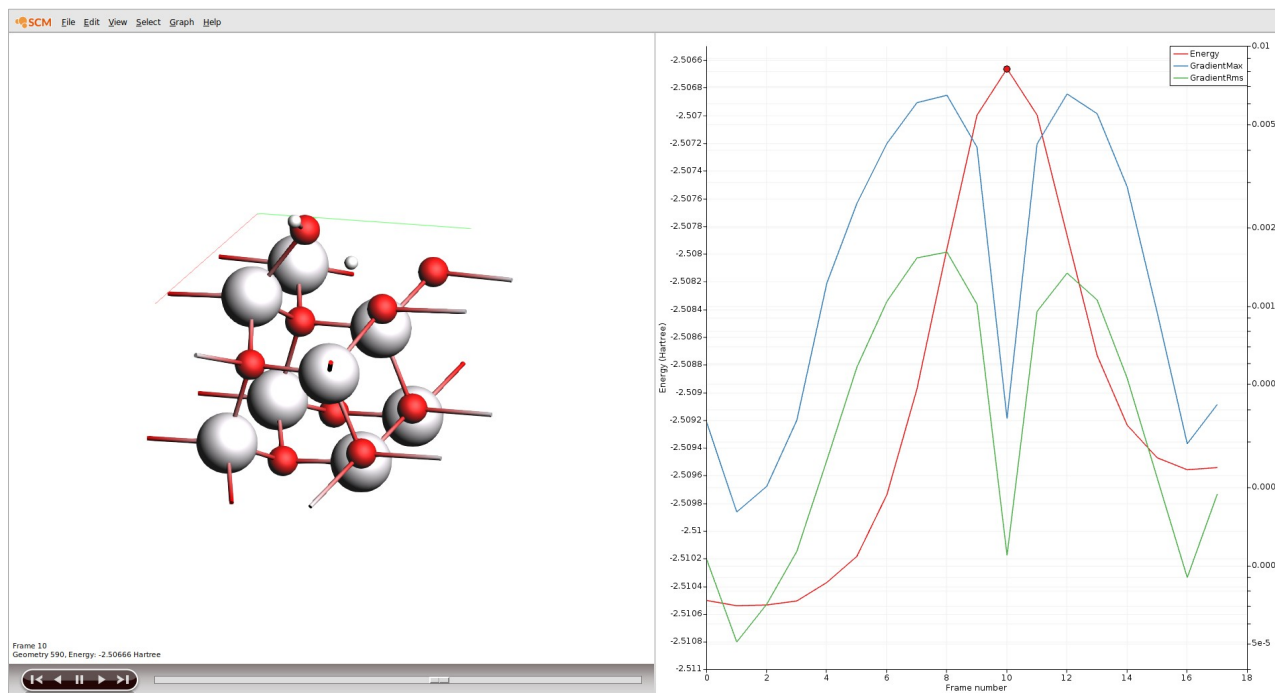


The screenshot shows the 'Nudged Elastic Band (NEB)' configuration panel within the 'ReaxFF' software. The panel is divided into several sections with various input fields and checkboxes.

Parameter	Value	Units/Options
Maximum number of iterations:	<input type="text"/>	
Number of images:	16	
Initial system:	initial	▼
Final system:	final	▼
Intermediate system:	<input type="text"/>	▼
Spring value:	1.0	Hartree/Bohr ² ▼
Skewness:	1.0	
Interpolate in Internal coordinates:	<input checked="" type="checkbox"/> Yes	
Optimize reactants/products:	<input checked="" type="checkbox"/> Yes	
Climb highest image to TS:	<input checked="" type="checkbox"/> Yes	
CI force threshold:	0.0	Hartree/Bohr ▼
Characterize PES point:	<input type="checkbox"/> Yes	
Optimize lattice:	<input type="checkbox"/> Yes	
Jacobian value:	<input type="text"/>	
Convergence and optimization details 		
Restart from:	 <input type="text"/>	
Re-optimize reactants/products:	<input type="checkbox"/> Yes	
Use old tangent:	<input type="checkbox"/> Yes	
Map atoms to cell:	<input checked="" type="checkbox"/> Yes	

NEB Reaction Path



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

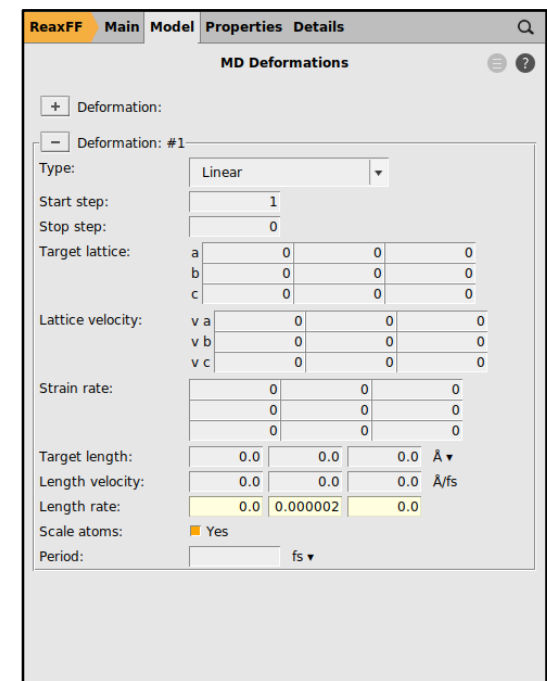


- ▶ **SCM** → **Spectra** to confirm the correct reaction mode

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>