



Chemistry & Materials Science with the
Amsterdam Modeling Suite 2019

Hands-On Session Part 2 – Periodic Systems

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on Computational Chemistry
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Overview



- ▶ Handling periodic systems
- ▶ Hands-on exercises
 - ▶ **Electronic structure of PdS₂ slab models**
 - ▶ **Mechanical properties of polymers**: see example below & advanced tutorial "*Mechanical properties of epoxy polymers*"




Periodic Systems

- ▶ Import structures
- ▶ Prepare slab models

Crystal Structures

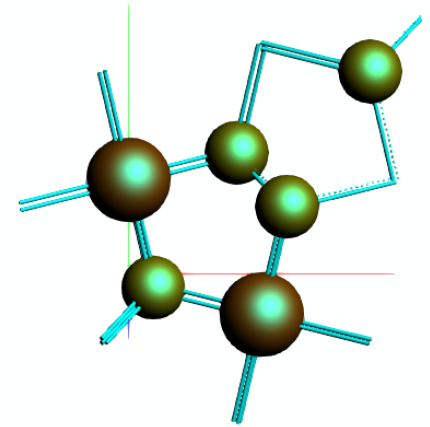


- ▶ Build from scratch in GUI:
periodic atomistic editor activates when using a periodic engine
- ▶ Amsterdam Modeling Suite template library: Access via  in GUI
- ▶ Load structure file via **File** → **Import Coordinates...**
 - ▶ From previous input (.adf) or output (.rkf) files
 - ▶ AMS internal format (i.e. xyz-file + lattice vectors)
 - ▶ .cif files from external sources like:
 - *crystallography.net*
 - *materialsproject.org*
 - article supporting information etc.

PdS₂ Crystal



- ▶ Preoptimized PdS₂ structure: import file `PdS2.cif` via **File** → **Import Coordinates...**
- ▶ Useful tools for periodic systems:
Edit → **Crystal** →
 - ▶ E.g. map atoms back to unit cell:
Edit → **Crystal** → **Map Atoms to (0..1)**

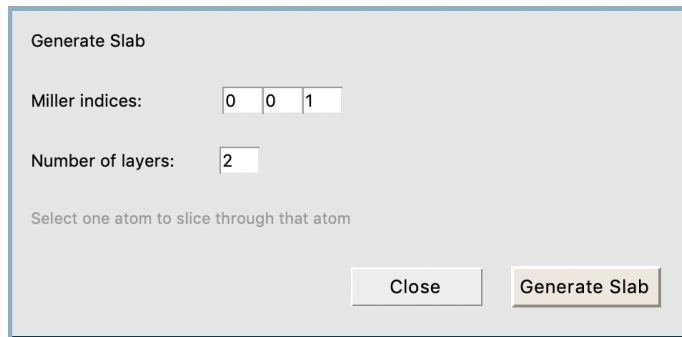


Number of atoms imported: 6, formula Pd2 S4

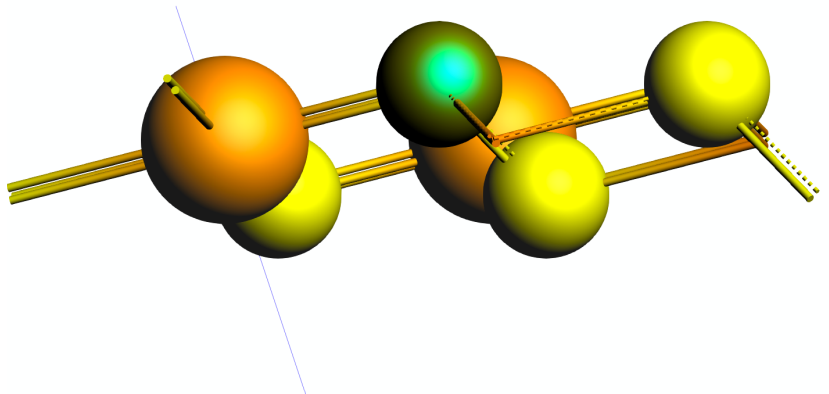
6 atoms selected

PdS₂ Slabs

- ▶ Create slab model:
 - ▶ `Edit` → `Crystal` → `Generate Slab...`



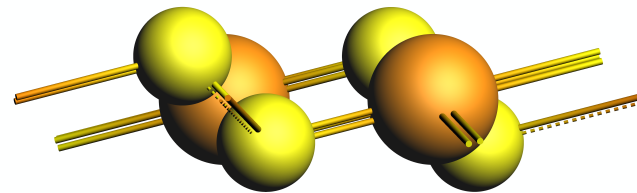
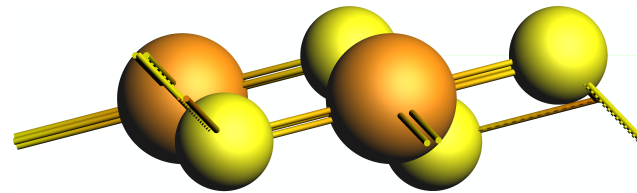
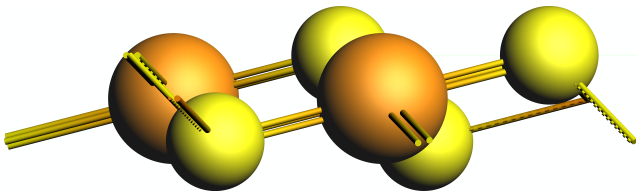
- ▶ Press `ctrl` + `1` to change perspective and select atom **S(4)**



- ▶ Click `Generate Slab`
- ▶ `File` → `Save as` → Enter `PdS2_Bilayer.adf`

PdS₂ Slabs

- ▶ Repeat with **Number of layers:** 1




- ▶ **File** → **Save as** → Enter PdS2_Monolayer.adf

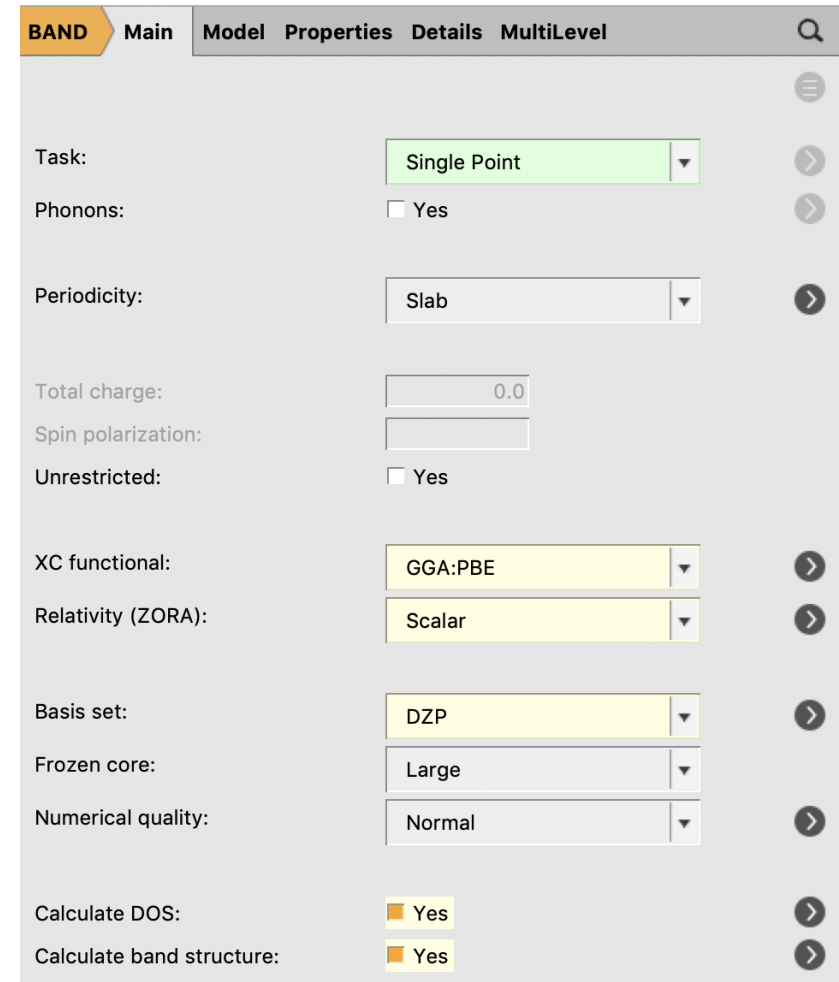


Band Structures

- ▶ Settings
- ▶ Band structure program
- ▶ DOS

Band Structure Settings

- ▶ Task: → Single Point
- ▶ XC functional → GGA → PBE
- ▶ Relativity (ZORA) → Scalar
- ▶ Basis Set: → DZP
- ▶ Tick Calculate DOS
- ▶ Tick Calculate band structure
 - ▶ Click on  next to it



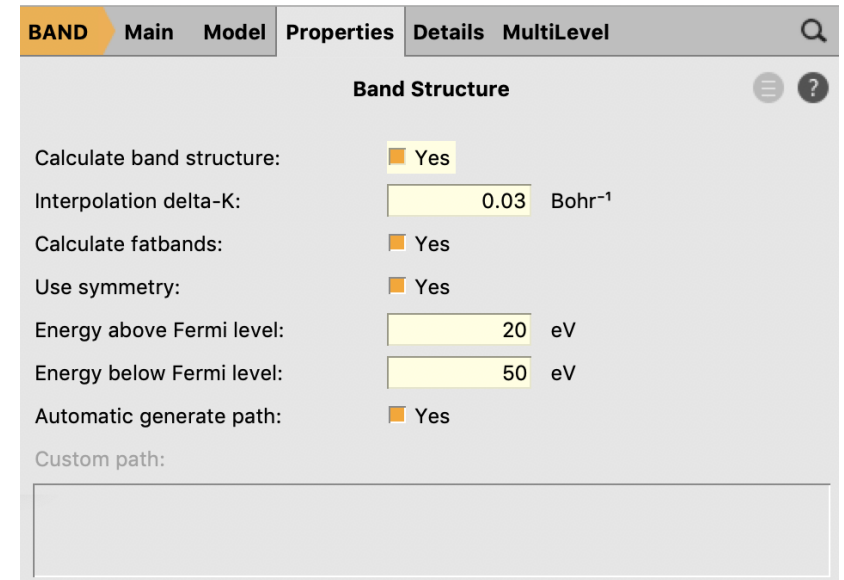
The screenshot shows the 'BAND' settings panel with the following configurations:

Parameter	Value
Task:	Single Point
Phonons:	<input type="checkbox"/> Yes
Periodicity:	Slab
Total charge:	0.0
Spin polarization:	
Unrestricted:	<input type="checkbox"/> Yes
XC functional:	GGA:PBE
Relativity (ZORA):	Scalar
Basis set:	DZP
Frozen core:	Large
Numerical quality:	Normal
Calculate DOS:	<input checked="" type="checkbox"/> Yes
Calculate band structure:	<input checked="" type="checkbox"/> Yes

Band Structure Settings




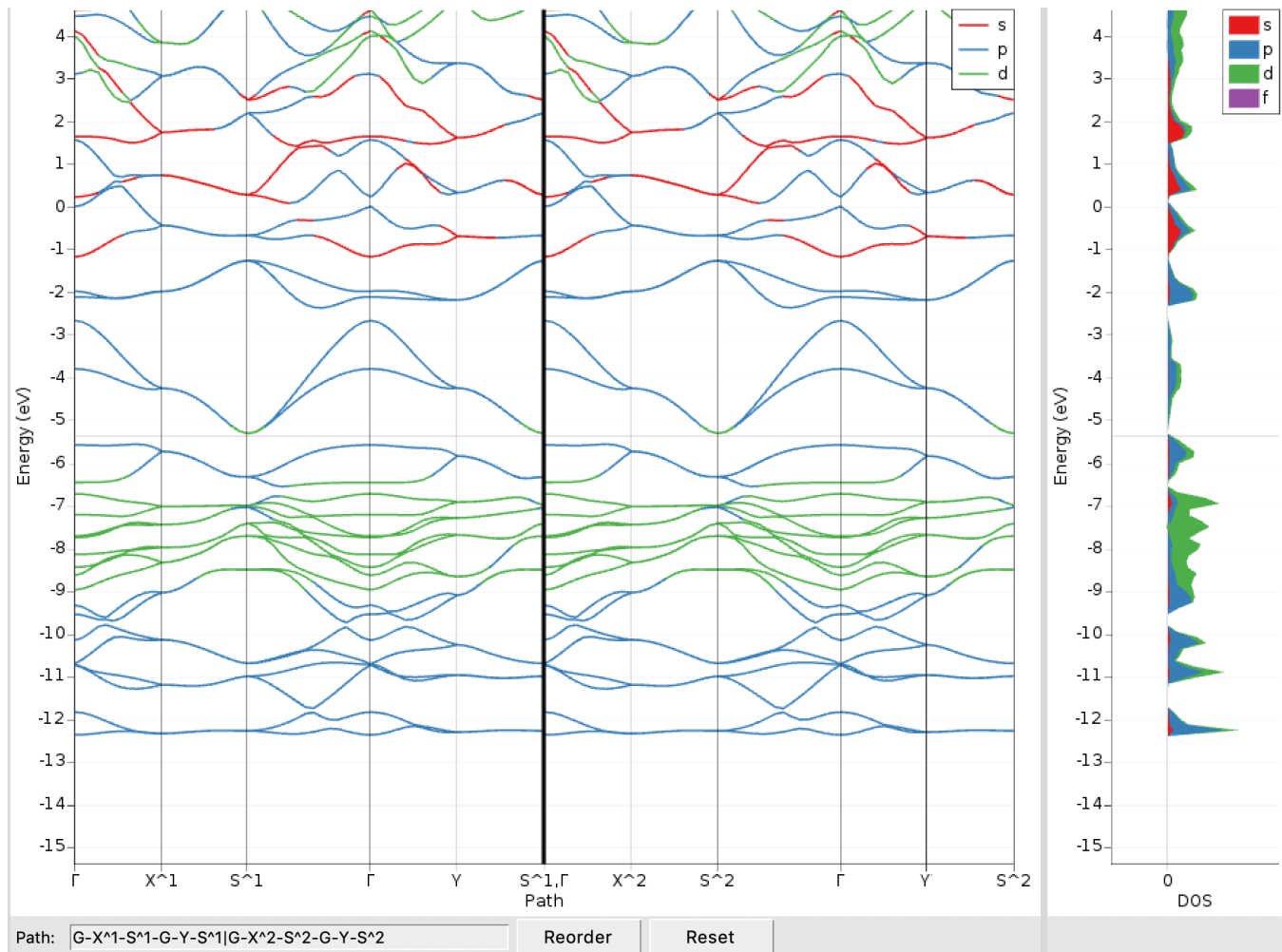
- ▶ Interpolation delta-K: $\rightarrow 0.03$
- ▶ Energy above Fermi level: 20 eV
- ▶ Energy below Fermi level: 50 eV



- ▶ Repeat for both systems and run calculations with **File** \rightarrow **Run**

Band Structure Analysis

- ▶ ADFjobs opens
- ▶ After calculations finish
 - ▶  → Band Structure

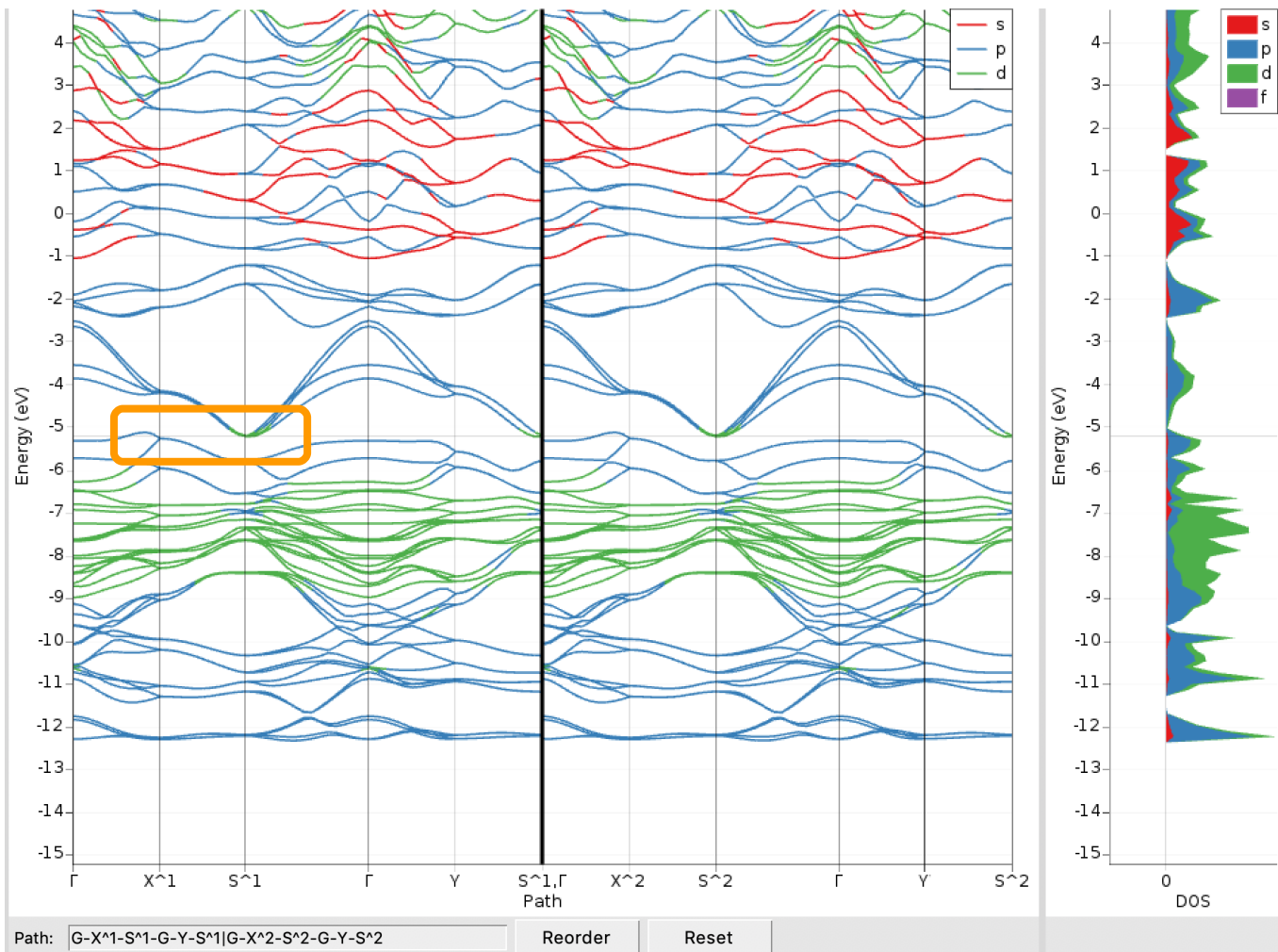


Band Structure Analysis

▶ Comparing both band structures:

- ▶ Semiconducting monolayer
- ▶ Conducting bilayer

“A Single-Material Logical Junction Based on 2D Crystal PdS₂”
M. Ghorbani-Asl, A. Kuc, P. Miró, T. Heine, Adv. Materials 28 (2016)





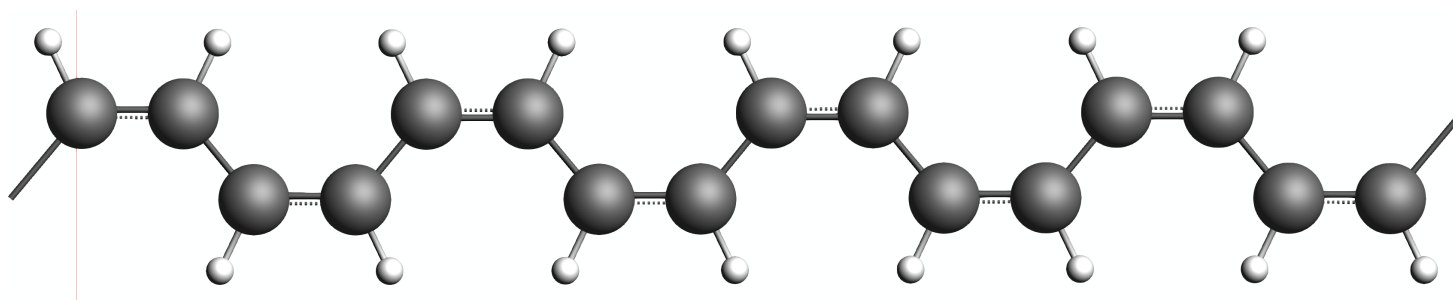
Mechanical Properties

- ▶ Small polymer toy system
- ▶ Stress-strain analysis
- ▶ Online version [here](#)
- ▶ Full-blown realistic [tutorial](#)

Example

▶ cis-Polyacetylene


- ▶ 3D periodic model in $19 \times 19 \times 19$ Å (required by ReaxFF)
- ▶ **File** → **Import Coordinates...**

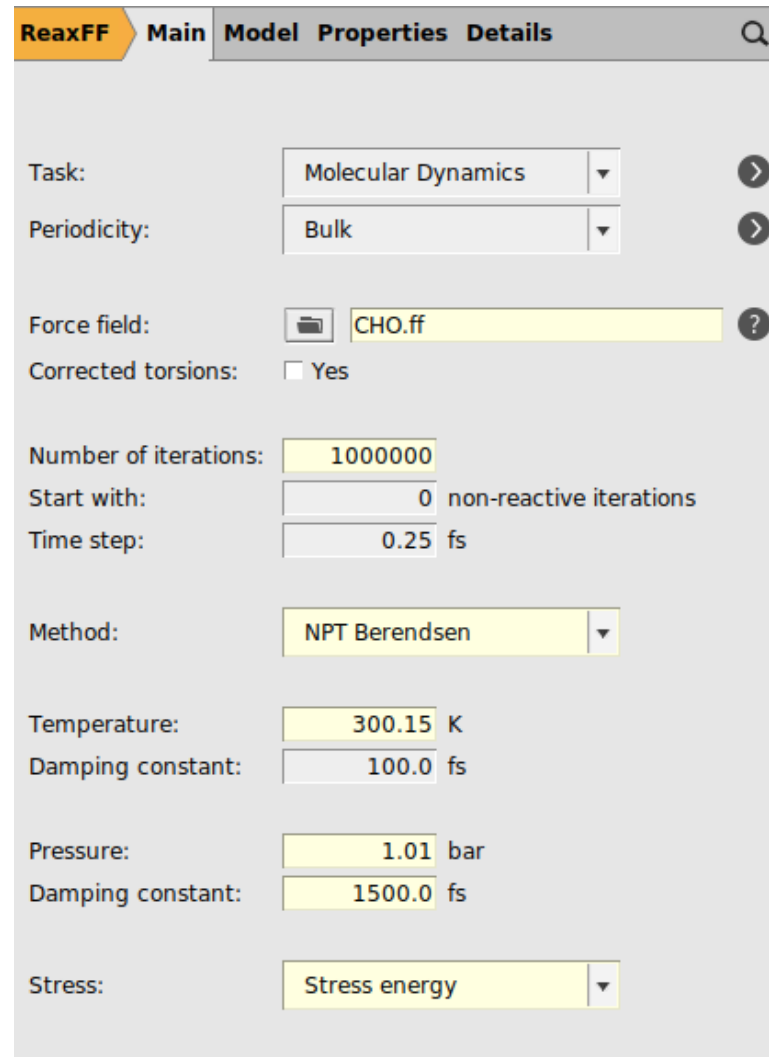


- ▶ Alternatively: Build from scratch (demo)
- ▶ Strain in z-direction: induces transition to trans-Polyacetylene
- ▶ Even more strain: polymer chain snaps

Setup MD Calculation



- ▶  → New Input
- ▶ File → Import Coordinates...
- ▶ Pick `cis_PA.xyz`
- ▶ Select ReaxFF
 - ▶ Force Field: `CHO.ff`
 - ▶ Number of iterations: `1000000`
 - ▶ Method: NPT Berendsen
 - ▶ Temperature: `300.15` K
 - ▶ Pressure: `0.101` MPa
 - ▶ Damping constant: `1500.0` fs
 - ▶ Stress: Stress energy




The screenshot shows the 'ReaxFF' configuration panel in the SCM software. The panel has a tabbed interface with 'Main', 'Model', 'Properties', and 'Details' tabs. The 'Main' tab is active. The configuration is as follows:

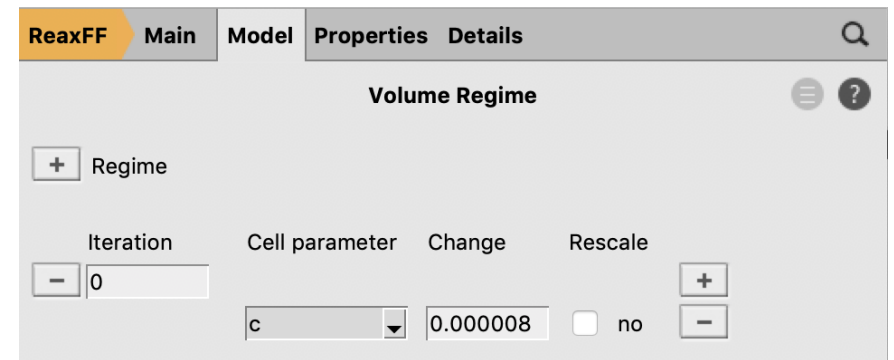
- Task:** Molecular Dynamics (dropdown)
- Periodicity:** Bulk (dropdown)
- Force field:** CHO.ff (file selector)
- Corrected torsions:** Yes
- Number of iterations:** 1000000
- Start with:** 0 non-reactive iterations
- Time step:** 0.25 fs
- Method:** NPT Berendsen (dropdown)
- Temperature:** 300.15 K
- Damping constant:** 100.0 fs
- Pressure:** 1.01 bar
- Damping constant:** 1500.0 fs
- Stress:** Stress energy (dropdown)

Strain Rate



- ▶ Details → Molecular Dynamics
 - ▶ Fix cell parameters (NPT only): c
 - ▶ Output frequency: **KF result file: 2000** (saves disk space)

- ▶ Model → Volume Regime
 - ▶ Click on 
 - ▶ Cell parameter: select c
 - ▶ Change: 0.000008



- ▶ See [Advanced Tutorial](http://www.scm.com) on www.scm.com for calculation of strain rate

Run & Evaluation



- ▶ **File** → **Save & File** → **Run**
- ▶ Use **ADFMovie** to see polymer change under strain
- ▶ After calculation is completed
 - ▶ Open console (via **Help** → **Terminal** or **Command Line**)
 - ▶ `startpython stress_strain_curve.py JOBNAME.rxkf`
- ▶ Plot **stress_zz** component against **strain_z**, e.g.:
 - ▶ Type `gnuplot`
 - ▶ `plot "stress-strain-curve.csv" using 3:6`

