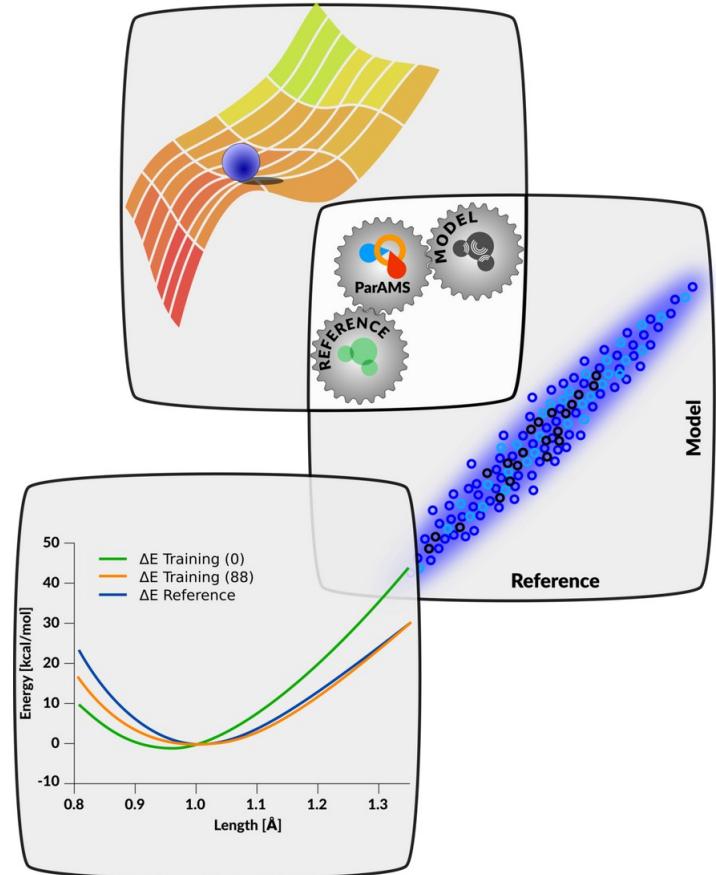


# ParAMS: ReaxFF and DFTB parameter optimization



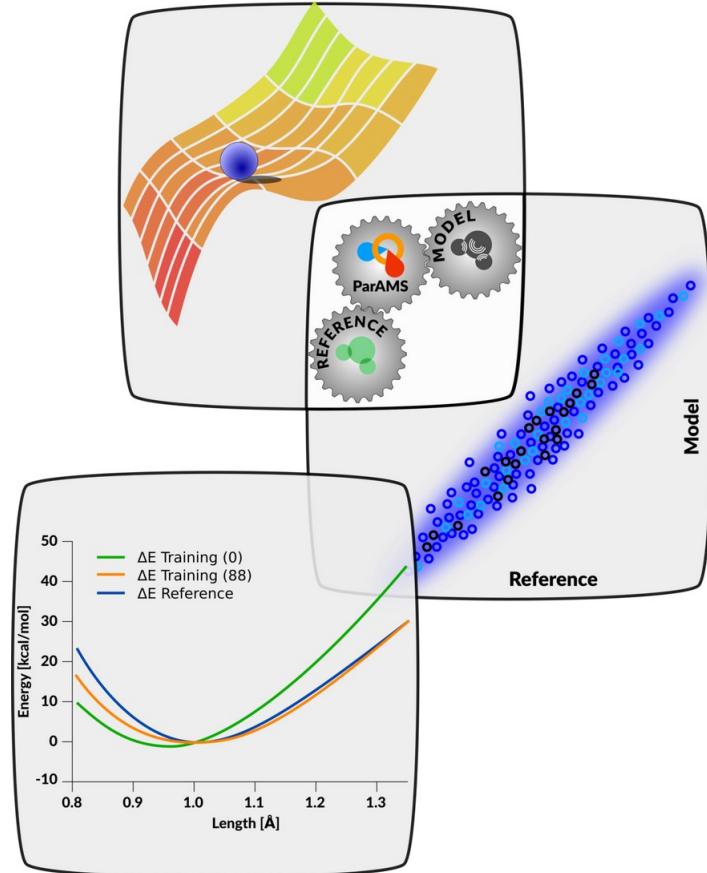
Matti Hellström, Product Manager

[hellstrom@scm.com](mailto:hellstrom@scm.com)



# Outline

- ▶ What is ParAMS?
- ▶ What can you do with ReaxFF and DFTB?
- ▶ Real-life ParAMS ReaxFF example from industry
- ▶ How does ParAMS work?
  - ▶ Add training data
  - ▶ Settings
  - ▶ Output
  - ▶ Various features
- ▶ Summary



# What is ParAMS?

- ▶ Optimize ReaxFF and DFTB (GFN1-xTB) parameters
- ▶ Collaboration with Prof. Toon Verstraelen, Ghent University, Belgium.
- ▶ Requires a license for “Advanced workflows and tools”, a new module in AMS2022
- ▶ ParAMS replaces the AMStrain module of previous AMS versions

## ParAMS: Parameter Optimization for Atomistic and Molecular Simulations

Leonid Komissarov, Robert Rüger, Matti Hellström, and Toon Verstraelen\*

 Cite this: *J. Chem. Inf. Model.* 2021, 61, 8,

3737–3743

Publication Date: May 13, 2021 ▾

<https://doi.org/10.1021/acs.jcim.1c00333>

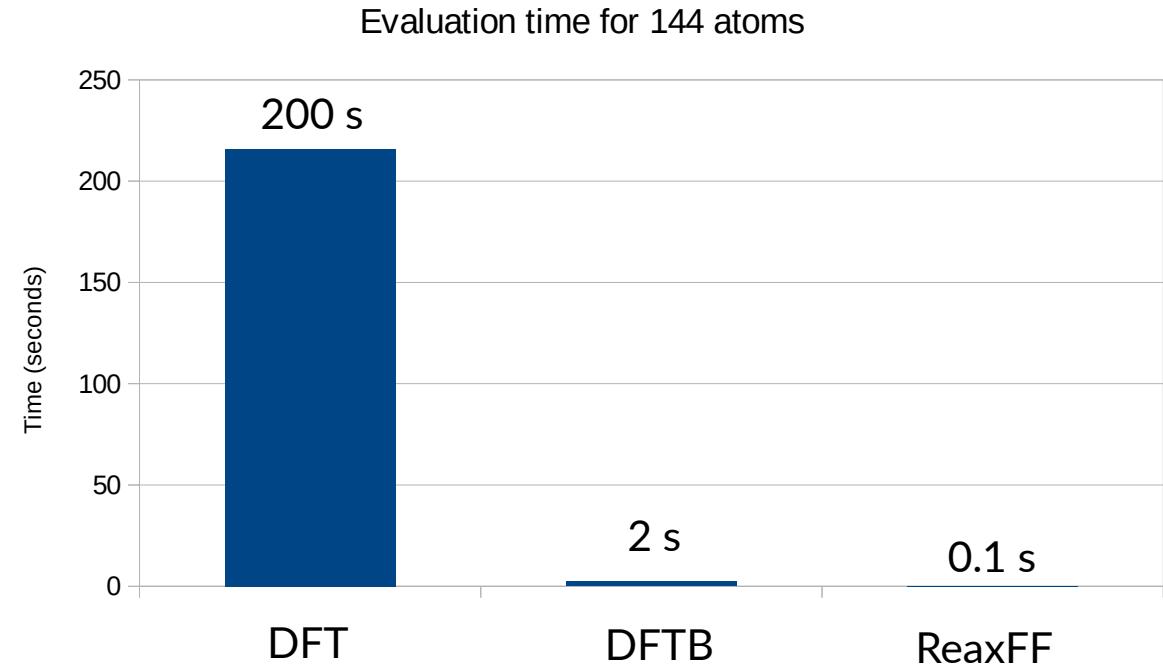
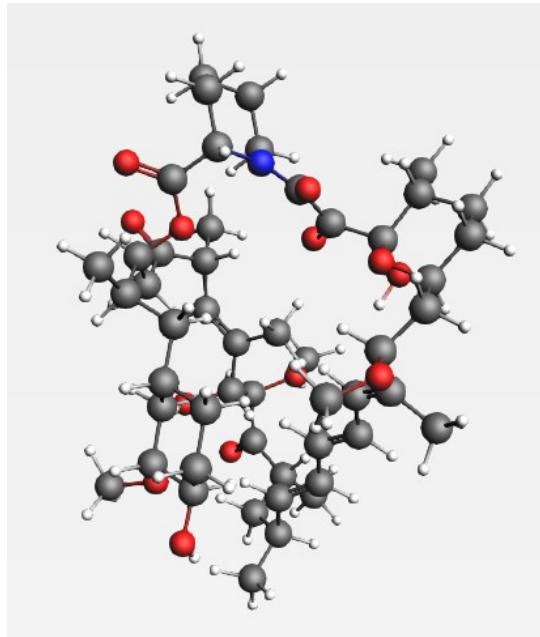
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# Why ReaxFF or DFTB?

- Faster than DFT



# Why are ReaxFF and DFTB faster than DFT?

- ▶ Parameters

- ▶ Example:

ReaxFF force field file

- ▶ ParAMS helps you

optimize the parameters

to give DFT-quality

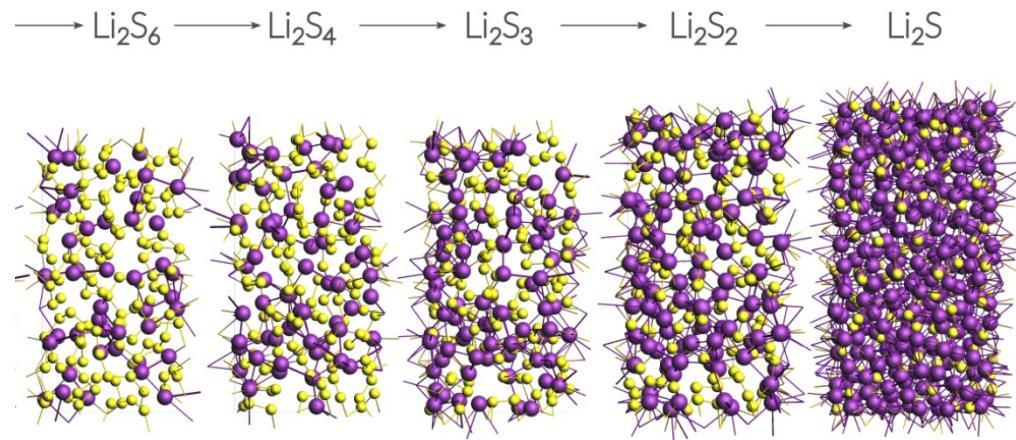
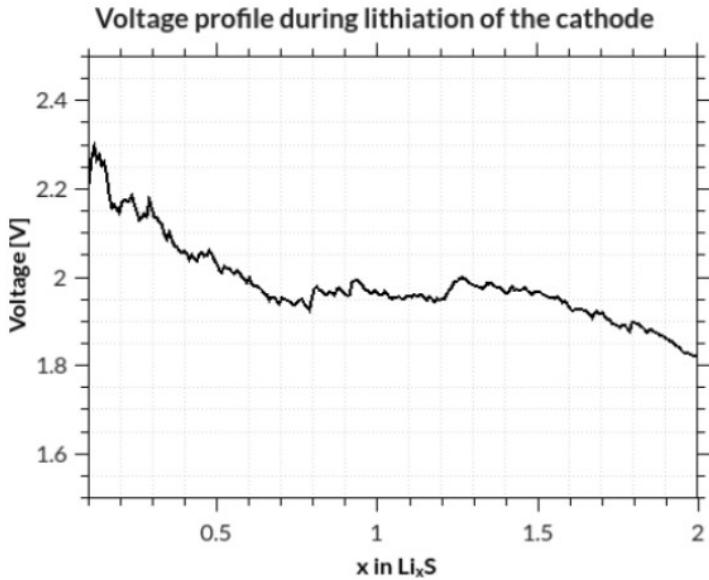
results

```

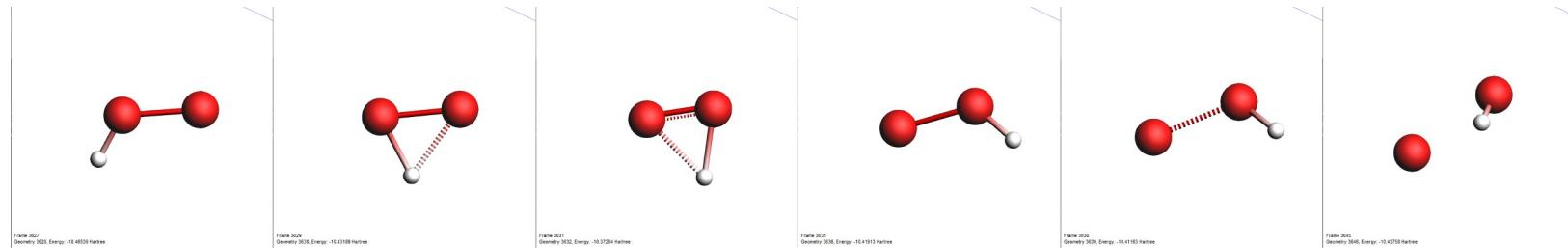
41      2.6962
42      0.0000
43      0.0000
44      3 ! Number of atoms
45
46
47
48      S    1.9186  2.0000  32.0600  1.6516  0.4937  0.7530  1.6593  6.0000
49      |  9.0227  4.9055  4.0000  30.0000 112.1416  6.5745  9.0000  2.0000
50      |  1.0000  3.4994 65.0000 12.0000 22.1978 15.3230  0.9745  0.0000
51      | -15.7363 2.8802  1.0338  6.2998  2.8793  0.0000  0.0000  0.0000
52      H    0.6646  1.0000  1.0080  1.6030  0.0600  0.7625 -0.1000  1.0000
53      |  9.3951  4.5386  1.0000  0.0000 121.1250  3.8196  9.8832  1.0000
54      | -0.1000  0.0000 -0.1339  2.5732  2.6456  3.1680  1.0698  0.0000
55      | -12.9330 3.0626  1.0338  1.0000  2.8793  0.0000  0.0000  0.0000
56      Zn   1.8862  2.0000  65.3900  1.9200  0.2998  0.4828 -1.6836  2.0000
57      | 11.5134 18.3776  2.0000  0.0078  0.0000  2.0219  5.7915  0.0000
58      | -1.2000  0.0000 266.4838  5.3430 10.1260  0.7590  0.0000  0.0000
59      | -3.0614  2.1158  1.0338  6.2998  2.5791  0.0000  0.0000  0.0000
60      6 ! Number of bonds
61
62      1  1  60.3691  31.1563  0.0000 -0.7739 -0.4781  1.0000 17.8574  0.3473
63      |  0.6134 -0.1773  8.4125  1.0000 -0.0909  6.1095  1.0000  0.0000
64      2  1 108.9303  0.0000  0.0000 -0.2724  0.0000  1.0000  6.0000  0.5333
65      |  4.3945  1.0000  0.0000  1.0000 -0.0984  4.6210  1.0000  0.0000
66      2  2 153.3934  0.0000  0.0000 -0.4600  0.0000  1.0000  6.0000  0.7300
67      |  6.2500  1.0000  0.0000  1.0000 -0.0790  6.0552  0.0000  0.0000
68      2  3  0.0000  0.0000  0.0000  0.0000 -0.5000  1.0000 50.0000  0.5000
69      |  0.5000 -0.5000 30.0000  1.0000 -0.2000  8.0000  0.0000  0.0000
70      3  3 31.5379  0.0000  0.0000 -0.7688 -0.2000  0.0000 16.0000  0.2229
71      |  0.3583 -0.2000 15.0000  0.0000 -0.0983  4.2268  0.0000  0.0000
72      1  3 112.1806  0.0000  0.0000 -0.3443 -0.5000  0.0000 35.0000  0.0346
73      |  1.1695 -0.5000 25.0000  0.0000 -0.3381  3.2746  0.0000  0.0000
74      0 ! Number of off-diagonal terms
75      6 ! Number of angles
76      1  1  1  70.3671  5.7180  7.0000  0.0000  0.3683  0.0000  2.4869

```

# AMS-ReaxFF: Li battery voltage profiles



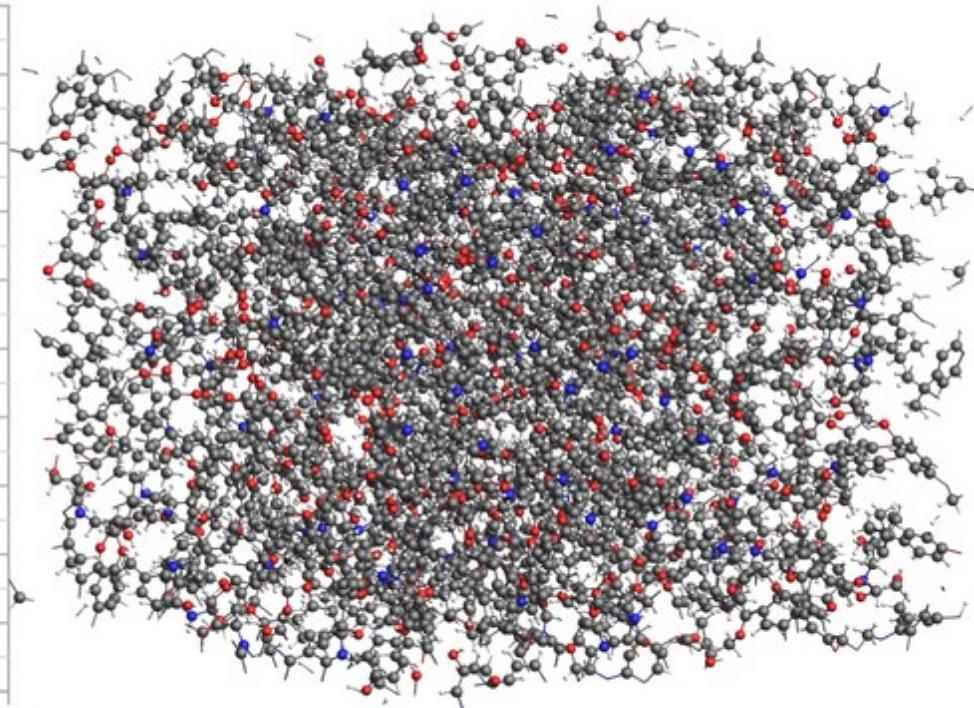
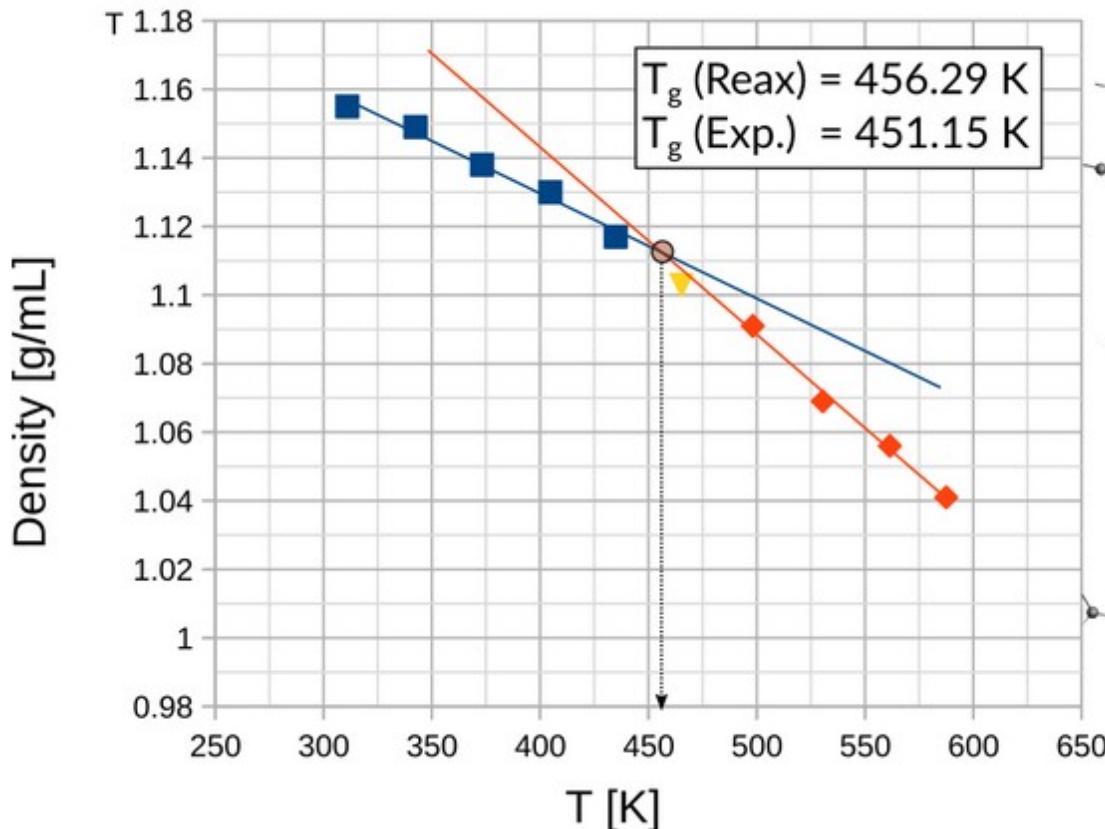
# AMS-ReaxFF: analyze reactive trajectories with ChemTraYzer2

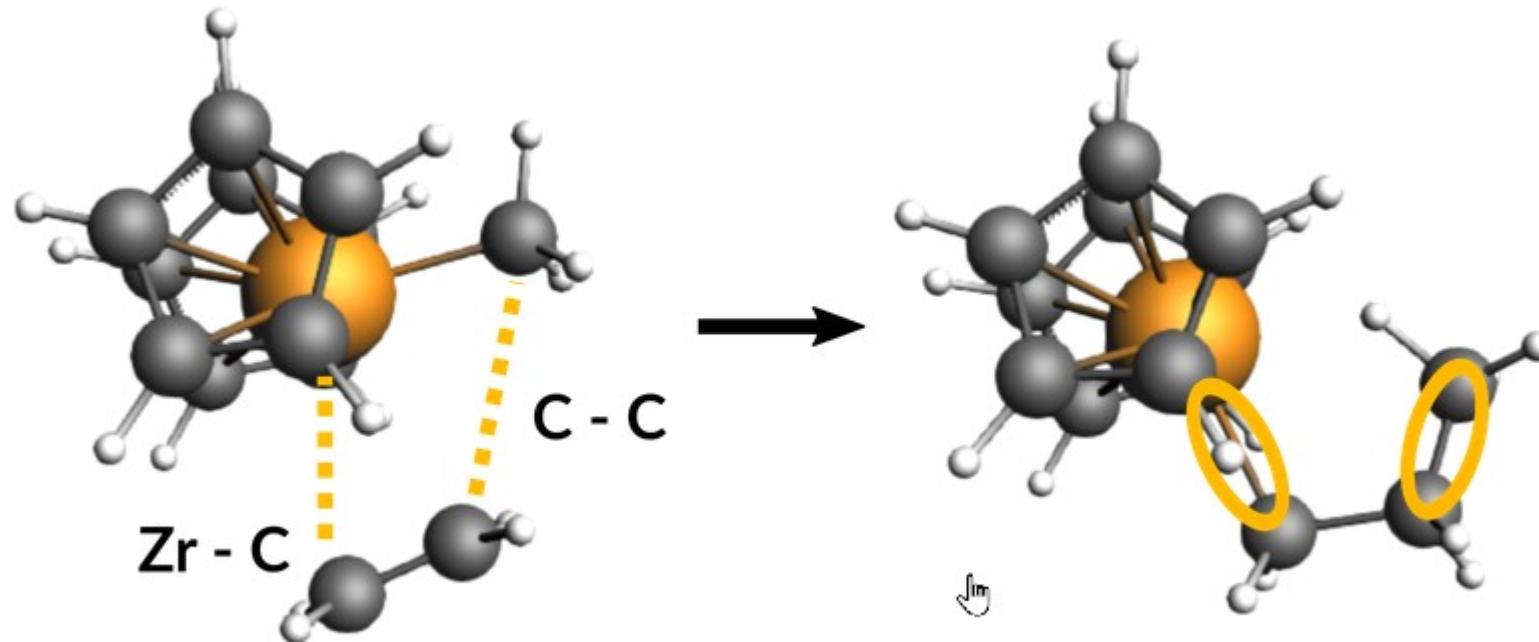


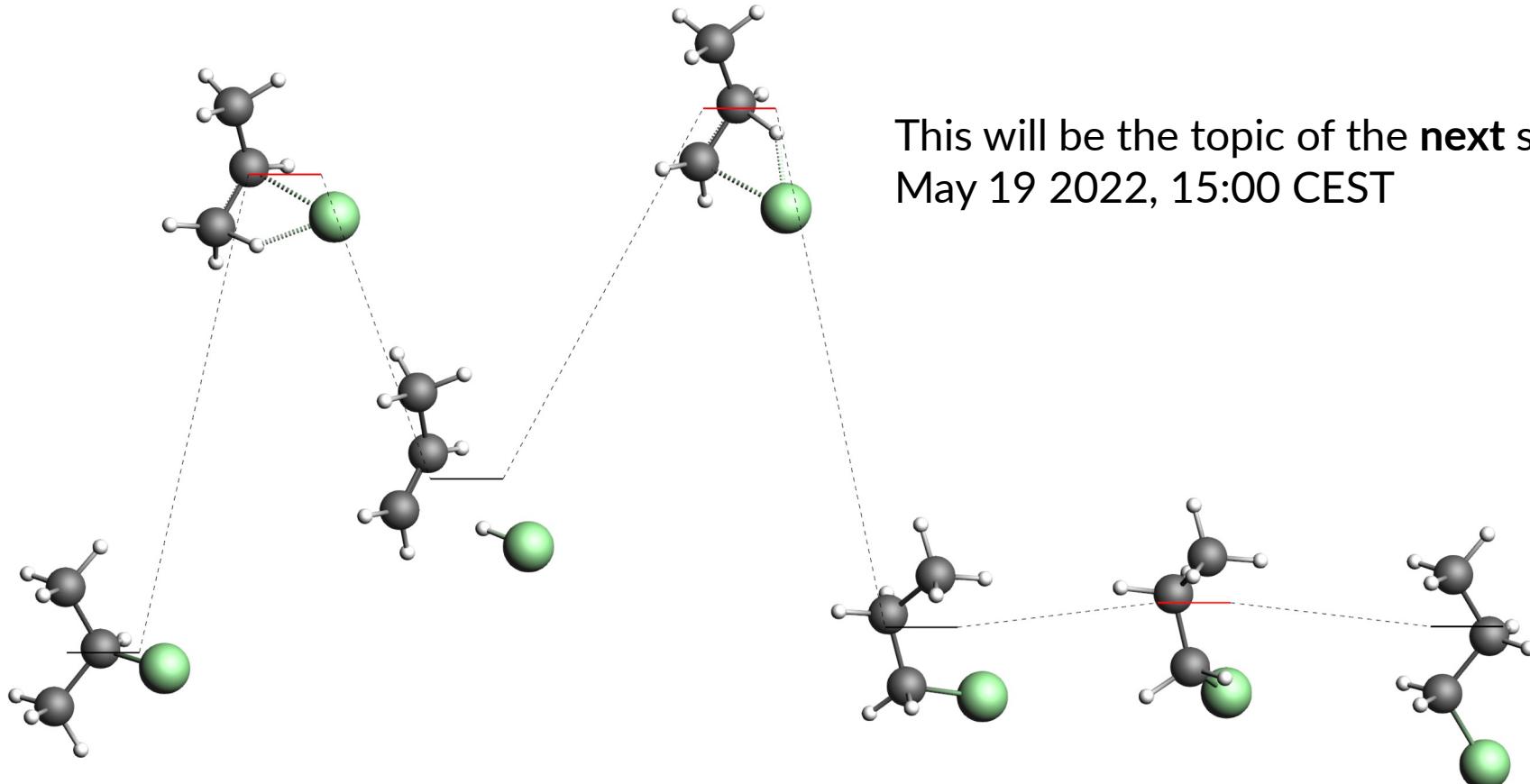
Reaction	Reaction Composition	Order	Rate constant k (cm <sup>3</sup> , mol, s)
$[O][O] + [H] \Rightarrow [O]O$	$O_2 + H \Rightarrow HO_2$	2	$1.407\text{e}+15$
$[O]O \Rightarrow [O][O] + [H]$	$HO_2 \Rightarrow O_2 + H$	1	$2.587\text{e}+12$
$[H][H] + [OH] \Rightarrow [H] + O$	$H_2 + HO \Rightarrow H + H_2O$	2	$3.881\text{e}+13$
$O[H]O \Rightarrow [OH] + O$	$H_3O_2 \Rightarrow HO + H_2O$	1	$4.072\text{e}+13$
$[H] + [OH] \Rightarrow O$	$H + HO \Rightarrow H_2O$	2	$1.903\text{e}+15$

Index	Initial frame	Final frame	Initial time (fs)	Final time (fs)	Reactants	Products
2	819	819	2047.5	2047.5	$[O]O$	$[O][O] + [H]$
5	894	894	2235.0	2235.0	$[O]O$	$[O][O] + [H]$

# AMS-ReaxFF: Polymer cross-linking and glass transition temperature







This will be the topic of the **next** seminar!  
May 19 2022, 15:00 CEST

## Step 1



- Optimize the structure of all molecules in the database with DFTB and calculate excitation energies and oscillator strengths with TD-DFTB
- Select the molecules with electronic excitations of energies between 1 and 6 eV and non-zero oscillator strength (since TD-DFTB is less accurate than TD-DFT, we opt for a larger energy range in this step). This should significantly reduce the number of molecules to be considered in the following steps.

## Step 2

- Optimize the structures of the promising molecules with ADF.
- Compute the electronic excitations energies using ADF's TD-DFT and select the molecules with excitations of energies between 2 and 4 eV (and non-zero oscillator strength).

<https://www.scm.com/doc/plams/examples/ExcitationsWorkflow.html>

# Preparametrized models in AMS

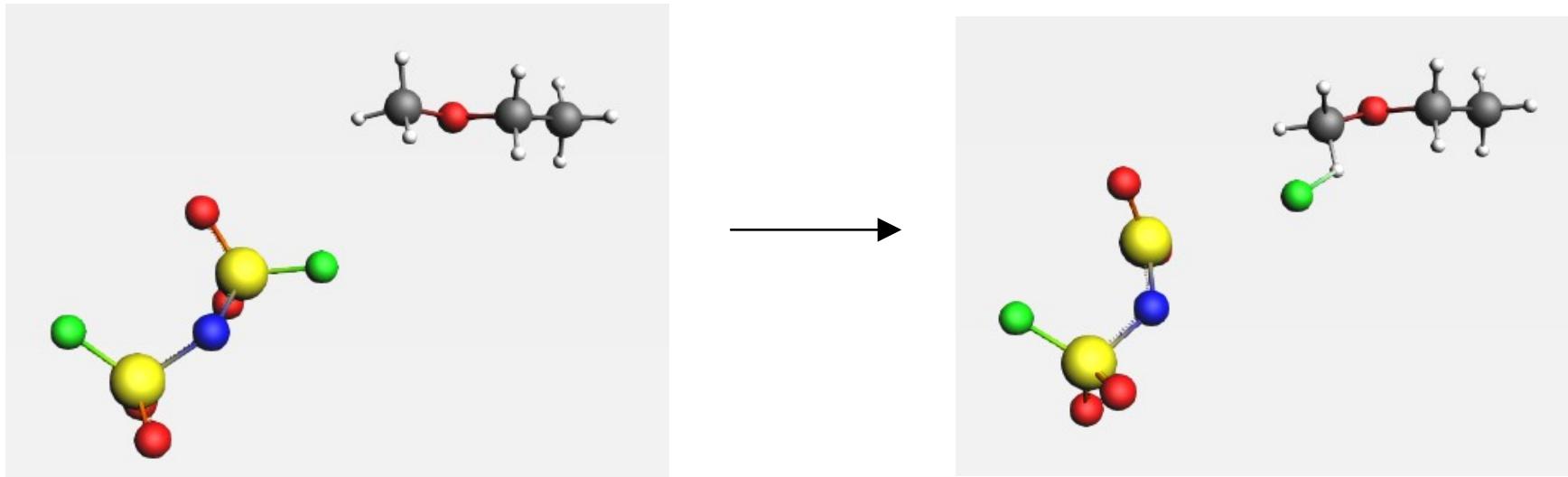
- AMS comes with many published ReaxFF force fields and DFTB parameters

Select Any File...	CHNa.ff AB.ff Ag-e.ff AgZnO.ff Al-H2O.ff AlCHO.ff AuCSOH.ff AuSCH_2011.ff AuSCH_2013.ff BaYZrCHO.ff C.ff CaSiAlO.ff CaSiOH.ff CBN.ff CeO.ff CH_aromatics.ff CHARHeNeKr.ff CHFe.ff	CHO-2016.ff CHO-radiation.ff CHO.ffd CHOAISI.ffd CHOCsKNaClIFLi.ffd CHOFe.ffd CHOFeAlNiCuS.ffd CHOFeAlNiCuScr.ffd CHOFeAlNiCuScr_v2.ffd CHOFeAlNiCuScr_v3.ffd CHOFeAlNiCuScrSiGe.ffd CHOGe.ffd CHOLi.ffd CHOLi_2.ffd CHOLiAlTiP.ffd CHON-2019.ffd CHON2017_weak.ffd CHON2017_weak_bb.ffd	CHONSFPtClNi.ffd CHONSi.ffd CHONSMgPNaCuCl.ffd CHONSMgPNaCuCl_v2.ffd CHONSMgPNaFBLi-e.ffd CHONSMgPNaTiClF.ffd CHONSMgPNaTiClFAu.ffd CHONSMgPNaTiClFKLi.ffd CHONSSI.ffd CHONSSI.ffd CHONSSI_CaCsKSrNaMgAlCu.ffd CHONSSI_Ge.ffd CHONSSI_Ge_2016.ffd CHONSSI_NaAl.ffd CHONSSI_NaFZr.ffd CHONSSI_NaP_tribology.ffd CHONSSI_NaP.ffd CHONSSI_PtNiCuCoZrYBa.ffd CHONSSI_PtZrNiCuCo.ffd	CHONSSIPtZrNiCuCoHeNeArKrXe.ffd CHONSZr.ffd CHOSFCIN.ffd CHOSiNa.ffd CHOSMoNiLiBFPN-2.ffd CHOSMoNiLiBFPN.ffd Co.ffd CsPbI.ffd CuBTC.ffd CuCHO.ffd CuCl-H2O.ffd CuSCH.ffd CuZr.ffd dispersion/CHONSSI-Ig.ffd FeOCHCl.ffd GaCH-2020.ffd Glycine.ffd HCONSB.ffd HE.ffd	HE2.ffd HONSiF.ffd HOSiAlLi.ffd HOSMg.ffd HOTiPd.ffd HSMo.ffd InCH-2020.ffd LiS.ffd LiSi.ffd Mue2016.ffd NaH.ffd NiCH.ffd NiCr.ffd OPT.ffd PdH.ffd PDMSDecomp.ffd PdO.ffd PtCH.ffd SiAlMgO.ffd	SiC.ffd SiOAlLi.ffd SiOH.ffd SiOHv2.ffd SiONH.ffd TiClOH.ffd TiO2bio.ffd TiOCHNCl.ffd undocumented/NiCH.f VOCH.ffd Water2017.ffd WSHAIO.ffd ZnOH.ffd ZrYOHVac.ffd ZrYONiH.ffd
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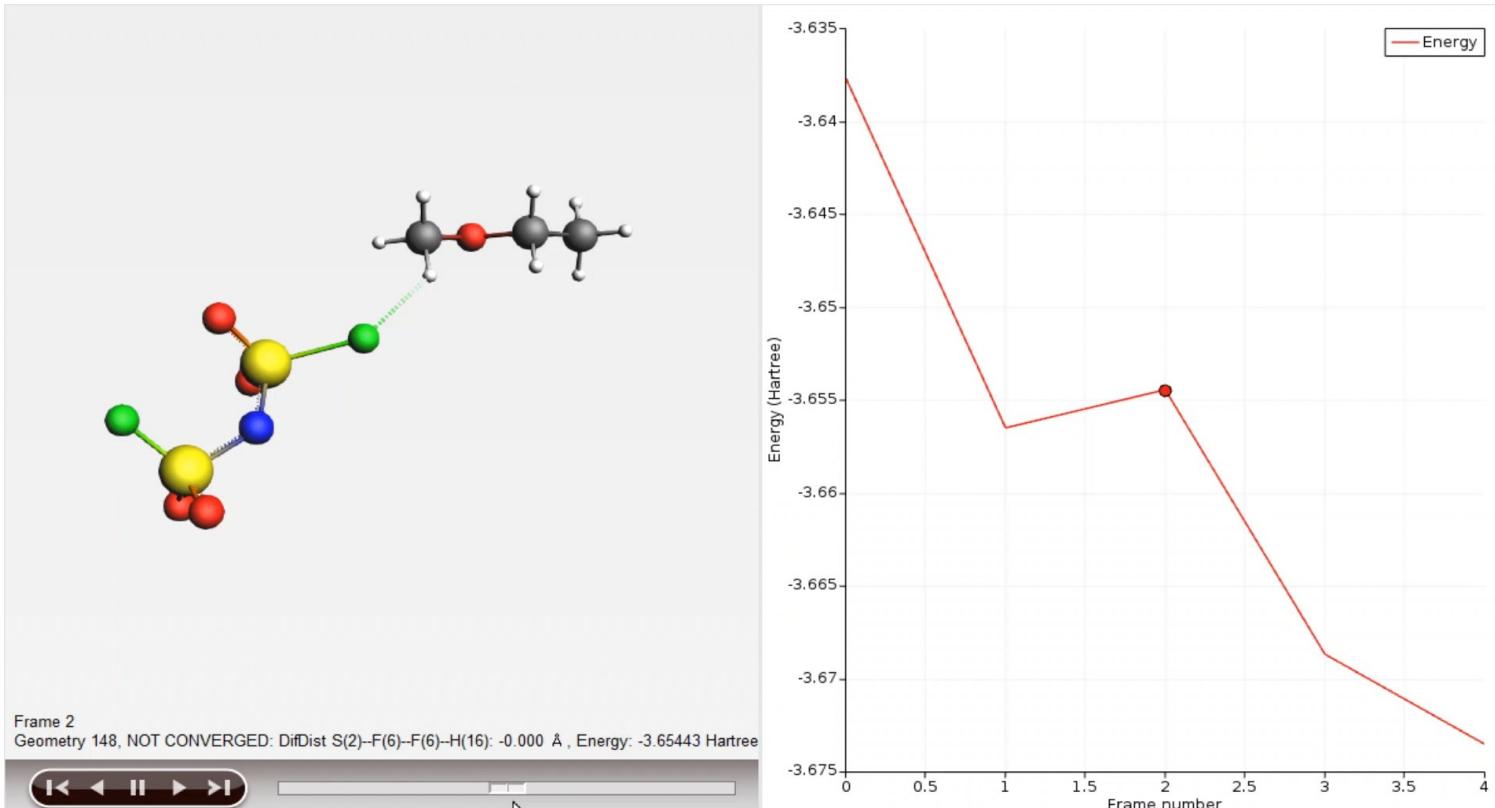
# ReaxFF and DFTB problems



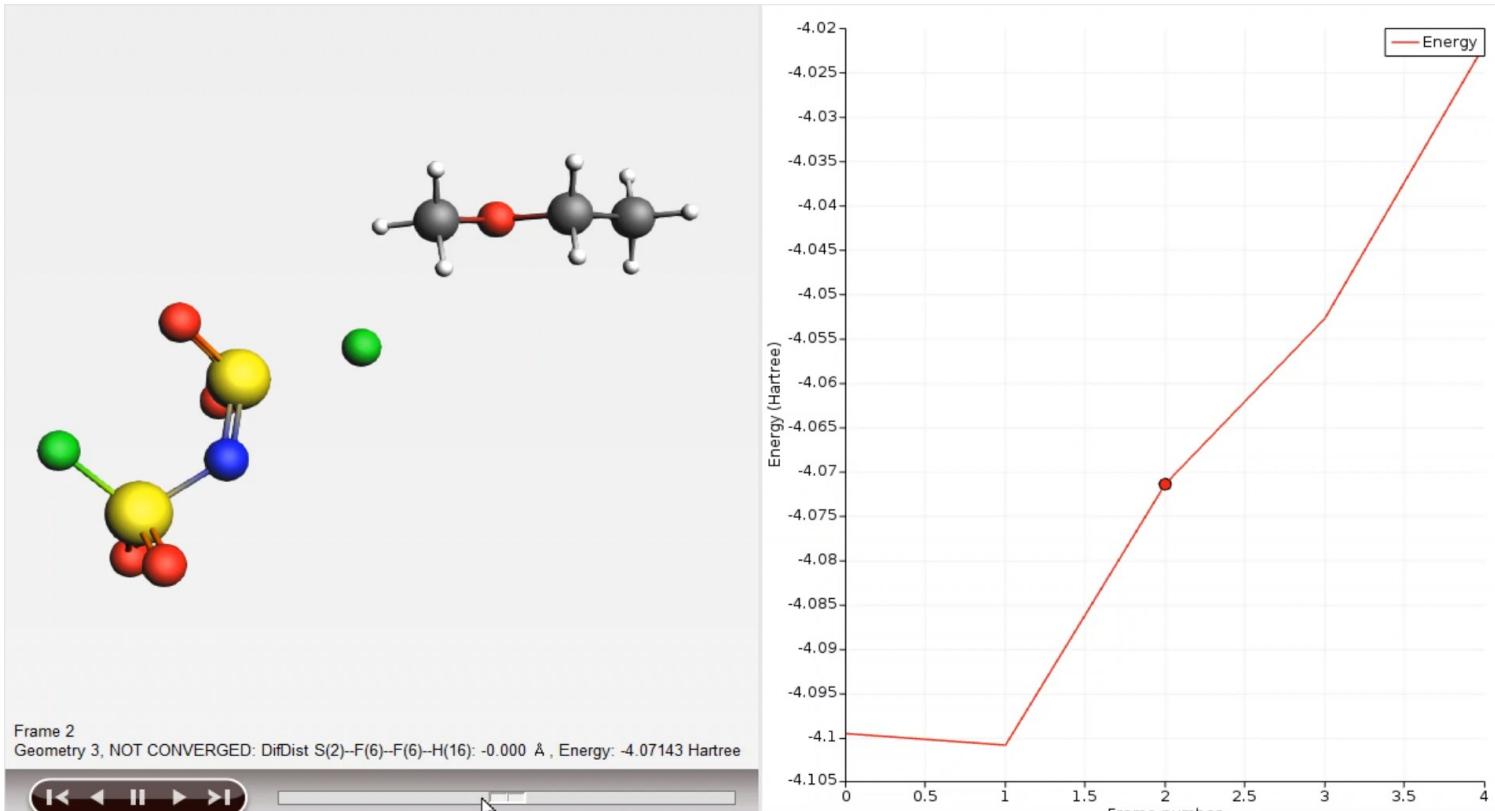
- ▶ They are not always accurate enough for “unseen” structures or molecules
- ▶ Example from an AMS industry customer: lithium bis(fluorosulfonyl)imide in organic solvent
  - ▶ Published ReaxFF force field predicts that a fluorine atom dissociates from the anion



# Published ReaxFF force field prediction



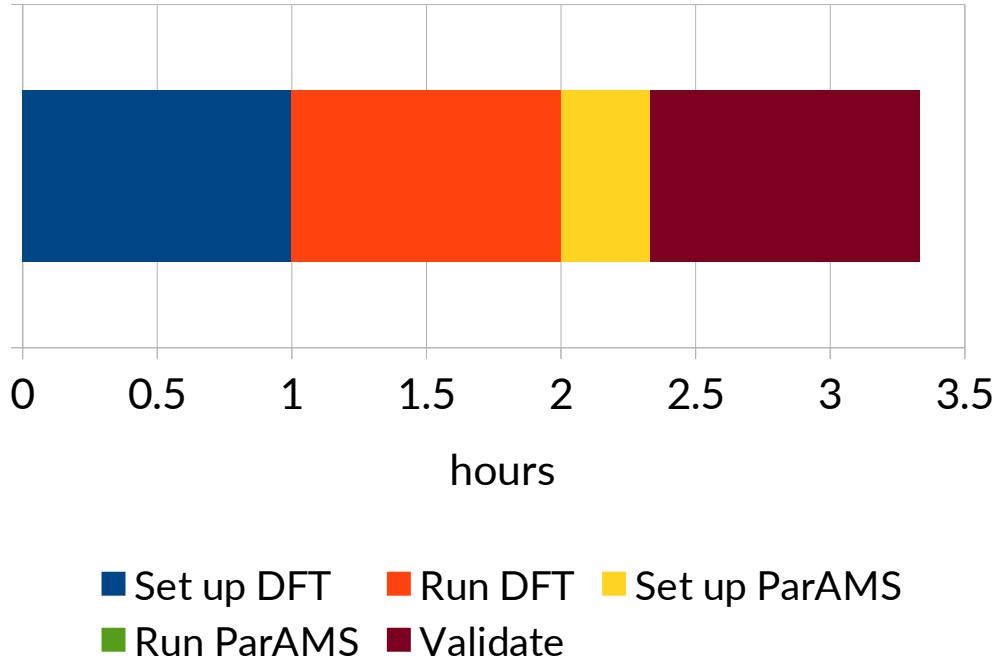
# AMS: Easily verify/disprove ReaxFF prediction with DFT



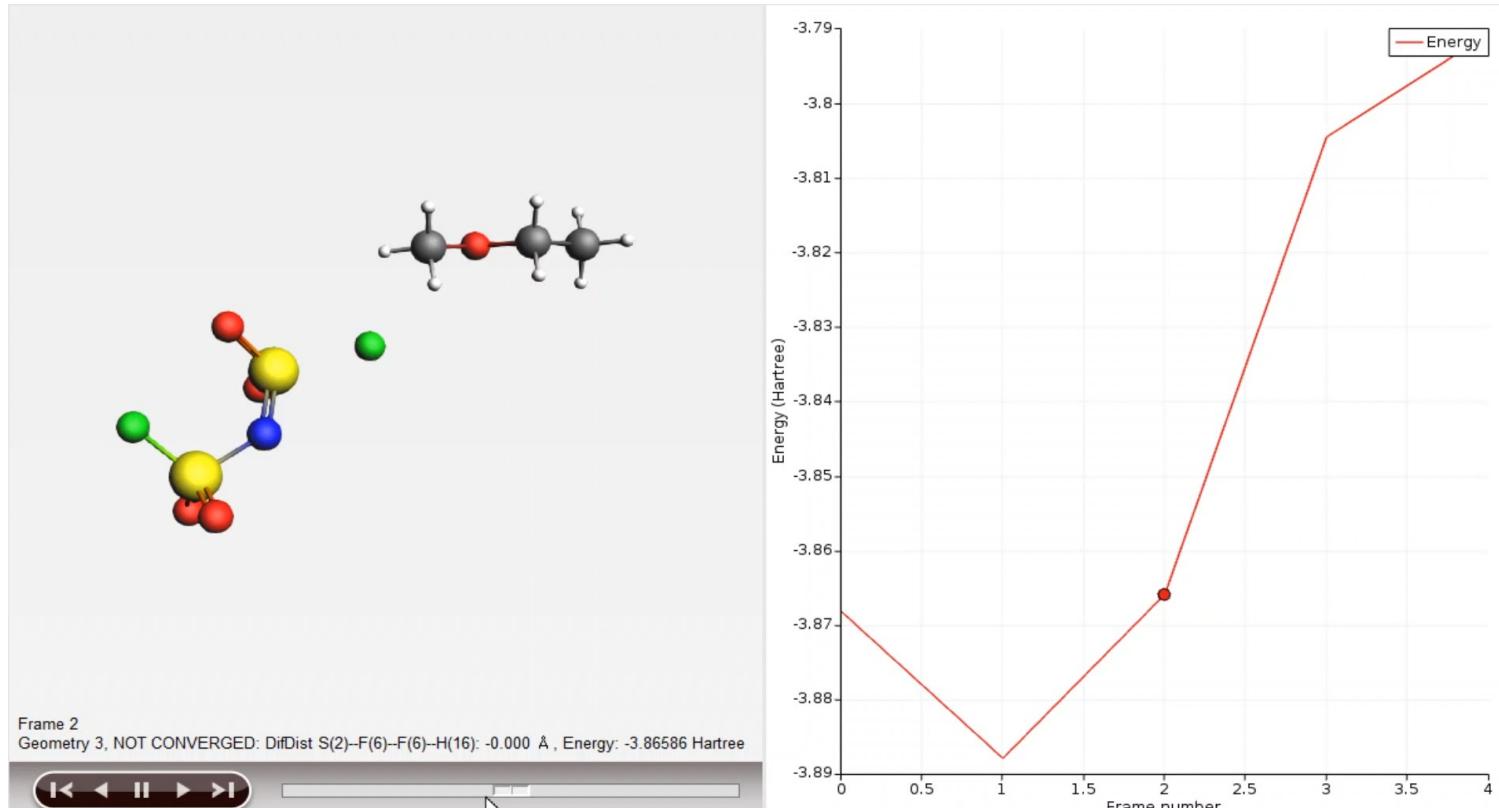
# AMS and ParAMS make it easy to fix the issue



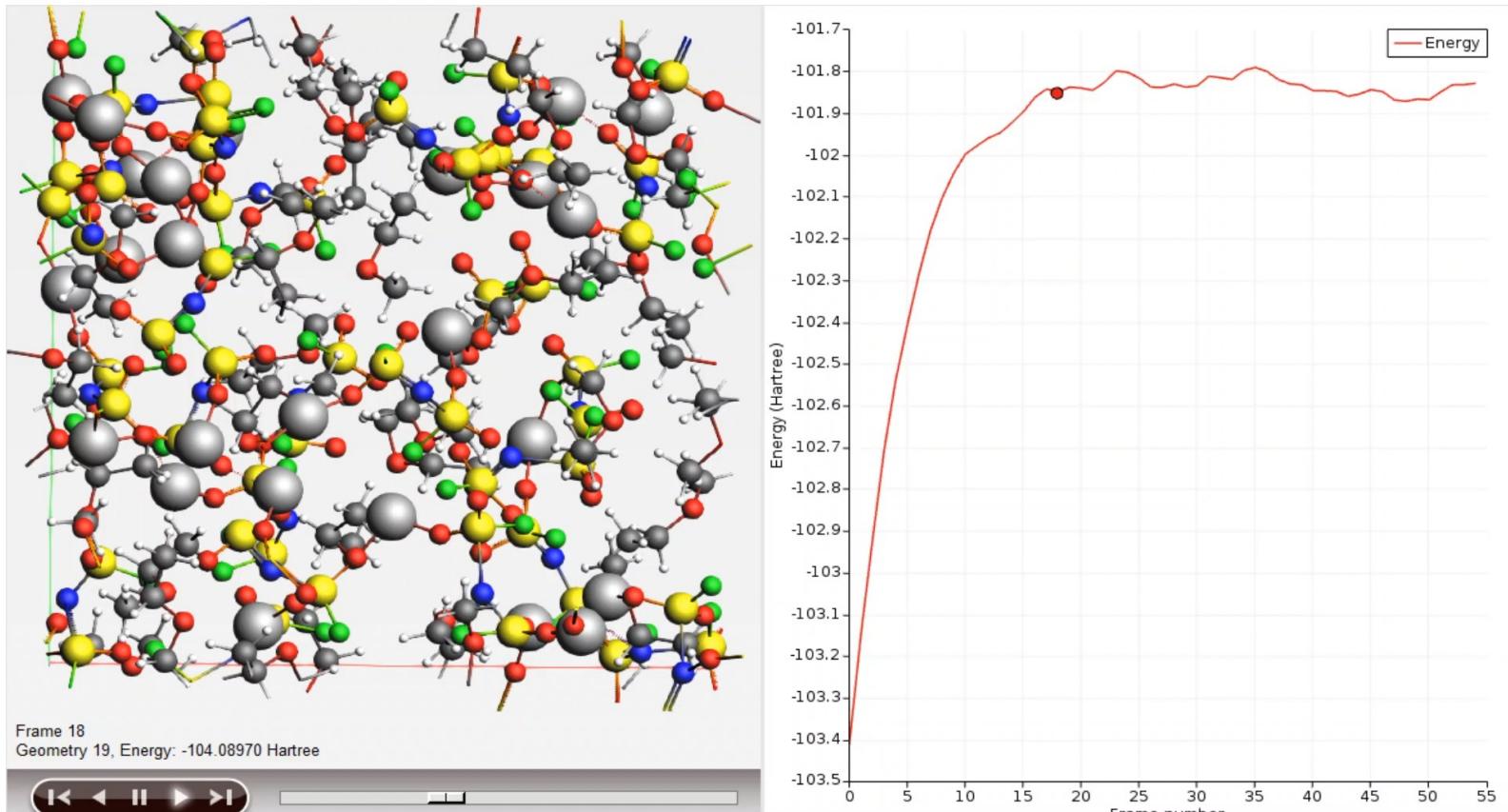
- ▶ For this example:
  - ▶ Set up new DFT calculations: 1 hour
  - ▶ Run DFT calculations: 1 hour
  - ▶ Set up ParAMS: 20 minutes
  - ▶ Reoptimize ReaxFF parameters: 10 seconds
  - ▶ Validate the new ReaxFF: 1 hour
- ▶ 0 lines of code! All steps supported by the graphical user interface.
- ▶ Note: Most parametrization projects will take longer



# Reoptimized ReaxFF predictions



# Production simulation



# General ParAMS workflow

- ▶ Validate an initial ReaxFF force field (if it exists)
- ▶ Set up new DFT calculations
- ▶ Run DFT calculations
- ▶ Set up ParAMS
- ▶ Run parameter optimization
- ▶ Validate new ReaxFF force field



iterative  
improvement

ParAMS minimizes the *loss function*

$$\sum_{i=1}^N w_i \left( \frac{y_i - \hat{y}_i}{\sigma_i} \right)^2$$

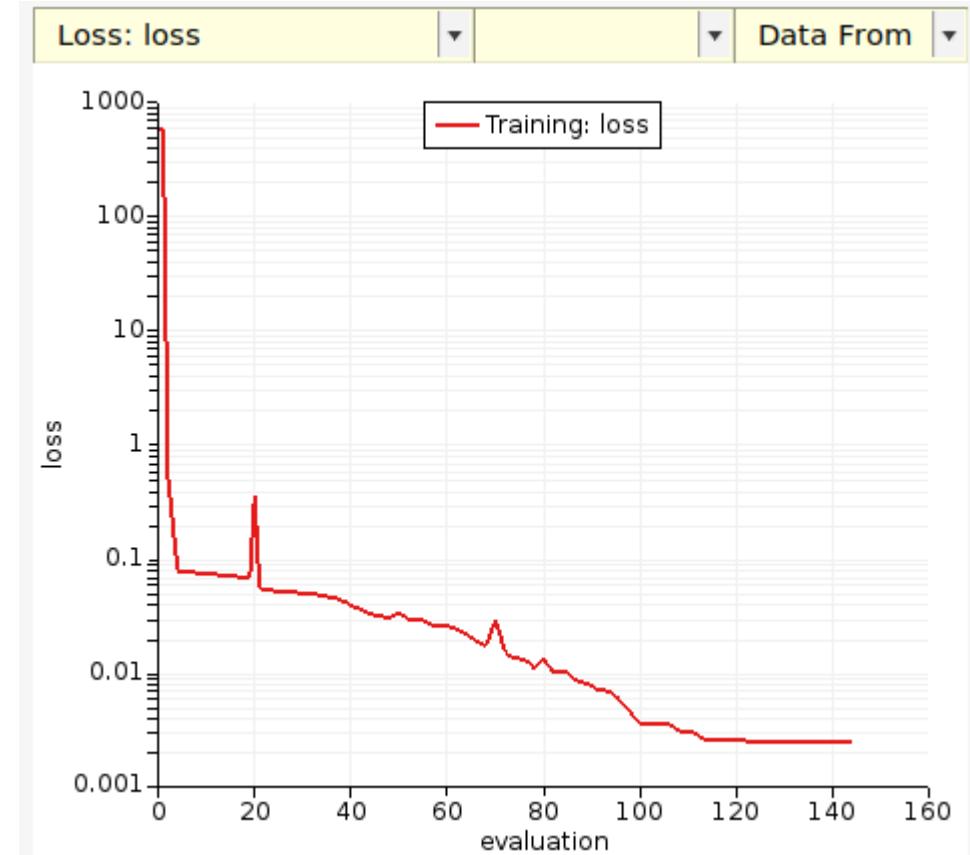
Training set size

Reference value

Predicted value

Weight

Unit normalization, "accuracy"

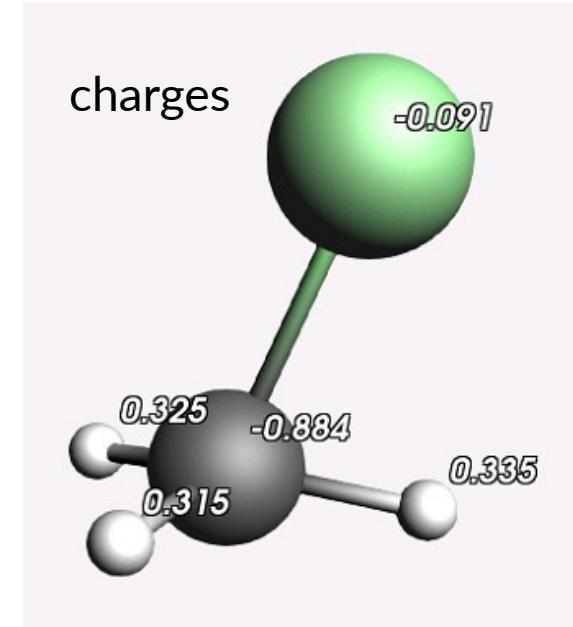
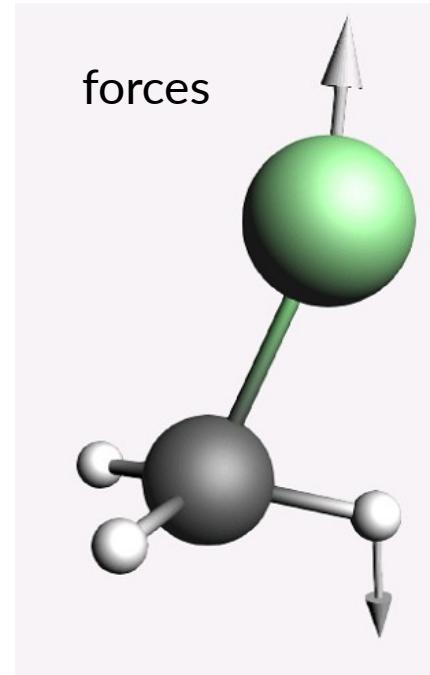


New parameters for every evaluation  
20

# ParAMS: Types of reference values



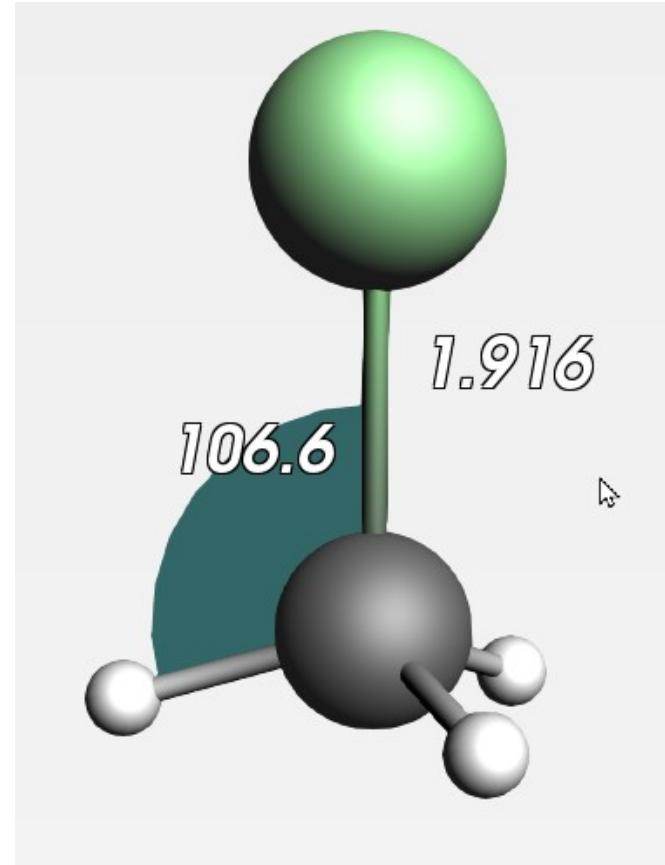
- ▶ “Anything” that can be extracted from a **job** can be used as a reference value
  - ▶ Forces, atomic charges



# ParAMS: Types of reference values



- ▶ “Anything” that can be extracted from a **job** can be used as a reference value
  - ▶ Optimized bond lengths or angles



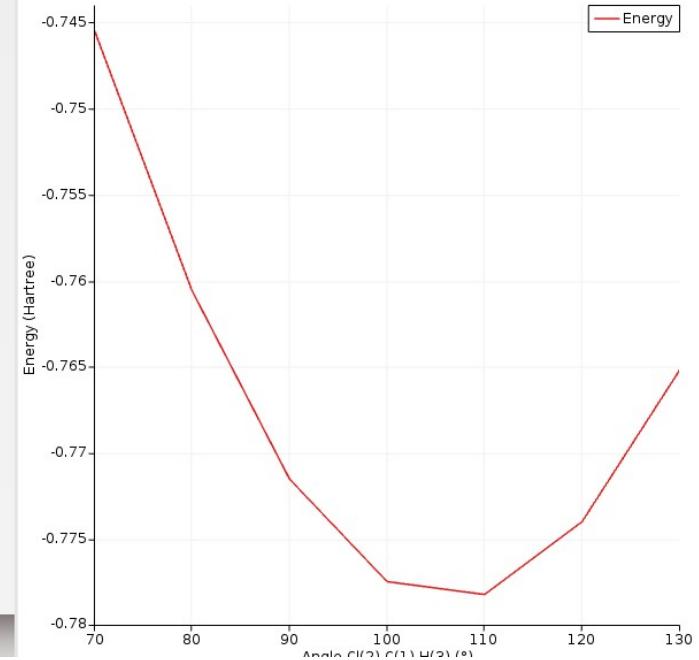
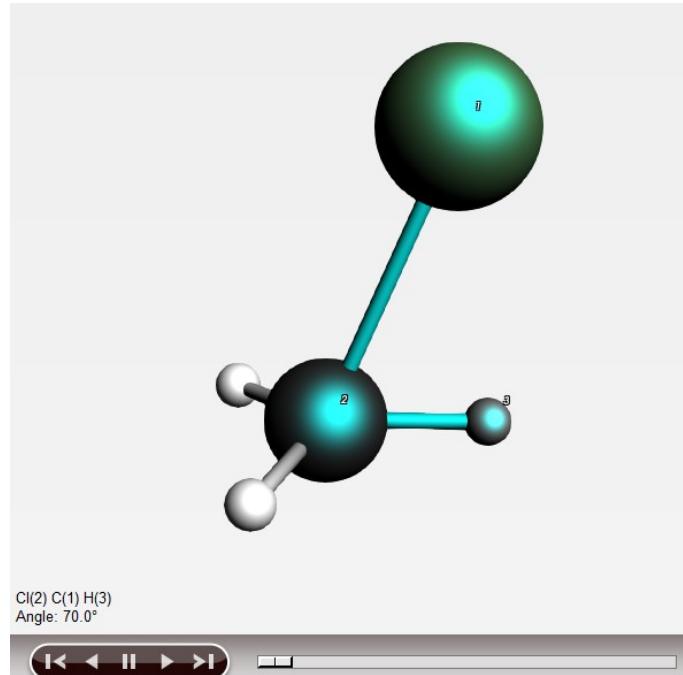
# ParAMS: Types of reference values



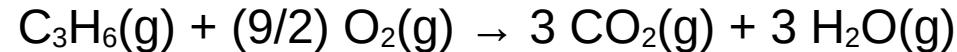
- ▶ “Anything” that can be extracted from a **job** can be

used as a reference value

- ▶ PES Scans:
  - Energy vs.
  - bond length,
  - angle, or
  - cell volume



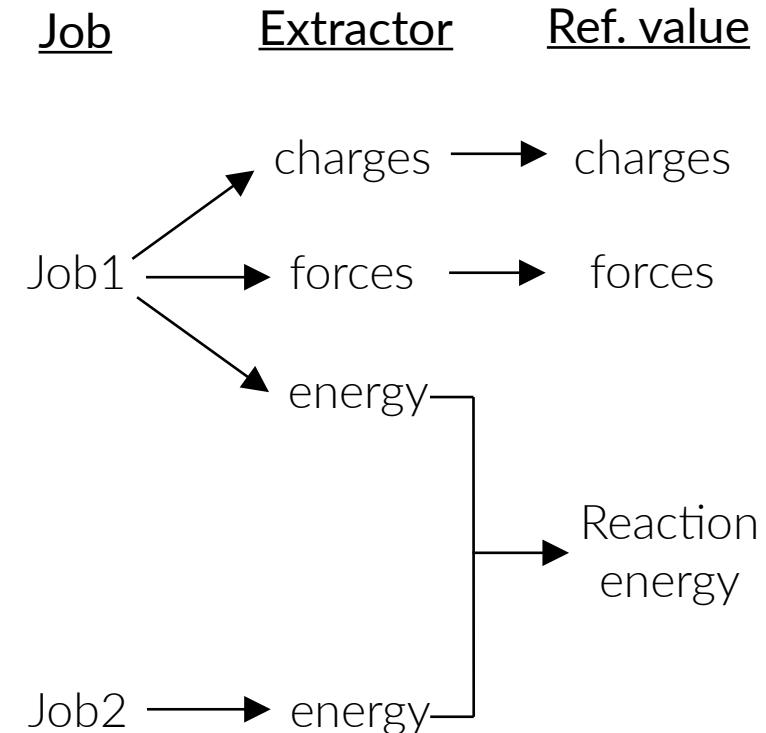
- ▶ Values from **multiple jobs**:
  - ▶ Reaction energies (adsorption energy, surface energy, formation energy, ...)



$$\Delta H_r^0 = -491.8 \text{ kcal/mol}$$

# ParAMS: Types of reference values

- ▶ “Anything” that can be extracted from a **job** can be used as a reference value
  - ▶ Forces, atomic charges
  - ▶ Optimized bond lengths or angles
  - ▶ PES Scans: Energy vs. bond length, angle, or cell volume
- ▶ Values from **multiple jobs**:
  - ▶ Reaction energies (adsorption energy, surface energy, formation energy, ...)

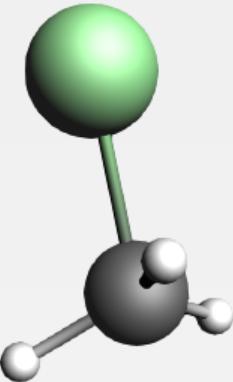


# Example reference values: Charges and forces of chloromethane



ParAMS 2022.101

SCM File Edit Jobs Parameters Training Set View Help



Job chloromethane-forces

All Jobs Training Set Validation Set Engines

Type	Detail	JobID	W	Value / Engines
Engine	Engine lennardjones EndEngine			ParAMS
Job	Single Point + gradients	chloromethane-forces		adf;;xc;;gga;PBE;
Charges	chloromethane-forces	chloromethane-forces	1.0	[-0.8835, 0.3345] (5) au
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;
Forces	chloromethane-forces	chloromethane-forces	1.0	[-0.1095, 0.0735] (5) Hartree/Bc

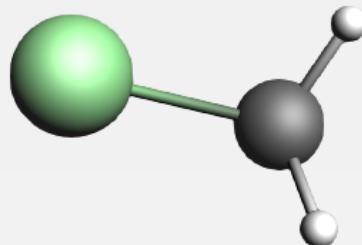
Parameters Settings Info **Graphs** Results

Weight:	+1.000000000		
Value:	-0.016768241	+0.018544396	-0.018888589
	+0.043055409	-0.109488031	-0.015582138
	-0.022345467	+0.073456592	+0.026842484
	-0.002046089	+0.011289727	+0.017385490
	-0.001895612	+0.006197316	-0.009757247

# Example reference values: Optimized bond lengths and angles



- ▶ For bond lengths and angles, add **geometry optimization** jobs!

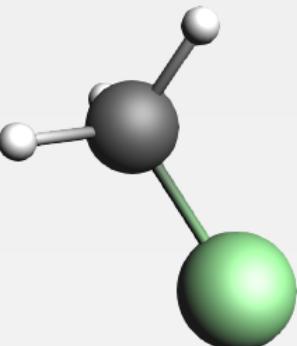


Type	Detail	JobID	W	Value / Engines
Engine	Engine lennardjones EndEngine			ParAMS
Job	Geometry Optimization + gradients + ...	chloromethane-geometry		adf;;xc;;gga;PBE;
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;
Geo: distanc	chloromethane-geometryoptimization, 0, 1 (C-Cl)	chloromethane-geometry	1.0	+1.91567508 Å
Geo: distanc	chloromethane-geometryoptimization, 0, 2 (C-H)	chloromethane-geometry	1.0	+1.09398928 Å
Geo: angle	chloromethane-geometryoptimization, 1, 0, 2 (Cl-C-H)	chloromethane-geometry	1.0	+106.60000000 °
Geo: angle	chloromethane-geometryoptimization, 2, 0, 3 (H-C-H)	chloromethane-geometry	1.0	+112.40000000 °

# Example reference values: Bond scan, angle scan, lattice scan



- ▶ For PES scans, add PES Scan jobs!



All	Jobs	Training Set	Validation Set	Engines
Type	Detail	JobID	W	Value / Engines
Engine	Engine lennardjones EndEngine			ParAMS
Job	PES Scan + gradients + ...	chloromethane-bondscan		adf;;xc;;gga;PBE;
PES	chloromethane-bondscan, relative_to=3	chloromethane-bondscan	1.0	[0.0000, 9.6074] (7) kcal/mol
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;

Job chloromethane-bondscan

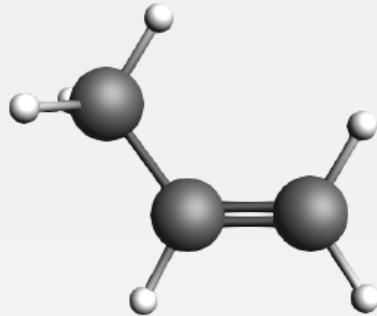
Parameters Settings Info Graphs Results

Weight: +1.0000000000

Value: +9.607422193 +4.075588043 +1.082804509 +0.0000000000 +0.348957323  
+1.763552064 +3.960264837

## Example reference values: Reaction energy

- ▶ Propene combustion:  $\text{C}_3\text{H}_6(\text{g}) + (9/2) \text{O}_2(\text{g}) \rightarrow 3 \text{CO}_2(\text{g}) + 3 \text{H}_2\text{O}(\text{g})$
- ▶ Automatically balanced stoichiometric coefficients!



Type	Detail	JobID	W	Value / Engines	
Engine	Engine lennardjones EndEngine			ParAMS	
Job	Geometry Optimization + ...	water		adf;;xc;;gga;PBE;	
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;	
Job	Geometry Optimization + ...	propene		adf;;xc;;gga;PBE;	
Job	Geometry Optimization + ...	co2		adf;;xc;;gga;PBE;	
Job	Geometry Optimization + ...	o2		adf;;spinpolarization;2;unr	
Engine	Engine adf spinpolarization 2 unrestricted yes xc gga PBE			adf;;spinpolarization;2;unr	
Energy	+3.0*co2+3.0*water-1.0*propene-4.5*o2	propene ...	1.0	-358.85844881	kcal/mol

► Which parameters to optimize?

- ▶ Choose as **few** as possible
- ▶ First try parameters in the “**standard**” category
- ▶ If a parameter value is close to min/max, change the range and continue

► Which optimization algorithm?

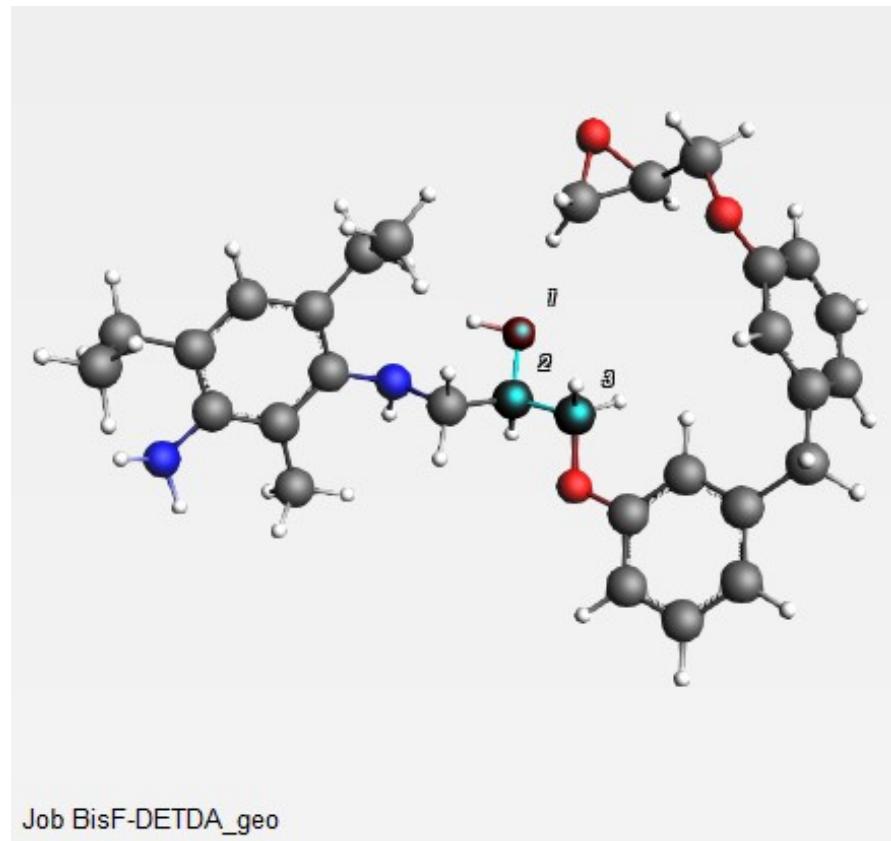
- ▶ We recommend **CMA-ES** for most optimization problems
- ▶ Details about this algorithm in previous seminar: <https://youtu.be/lcv7kWUaoTI>

Category	
Standard	Pi bond order parameter (eq. 2)
Standard	Pi bond order parameter (eq. 2)
Standard	Sigma bond order (eq. 2)
Standard	Sigma bond order (eq. 2)
DoNotOptimize	Uncorrected BO overcoordination (eq. 3a)
Expert	eReaxFF param for adjusting number of electr

# The ParAMS challenge 2022

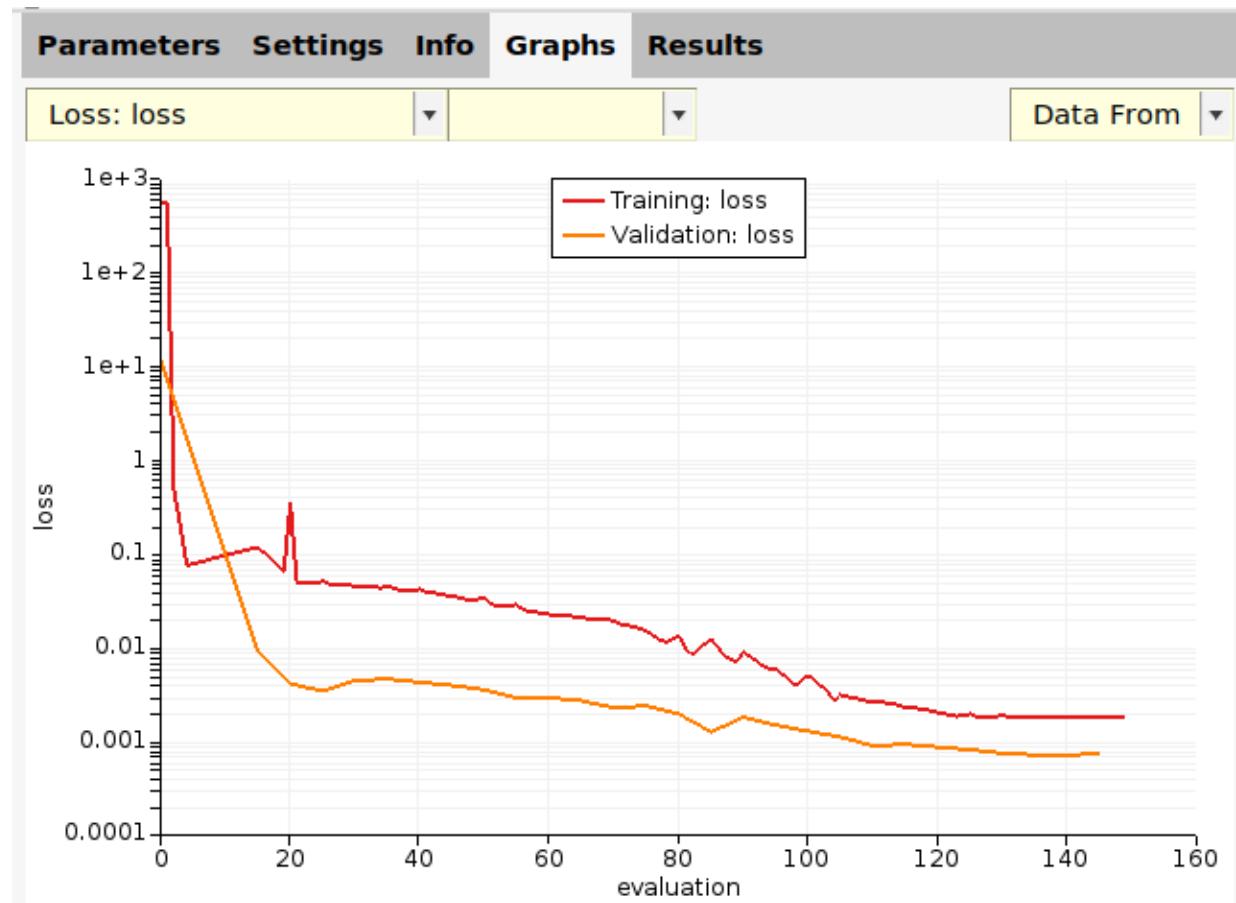


- ▶ Fit and submit a ReaxFF force field
- ▶ Hundreds of euros in **prizes**
- ▶ Reasonable input has already been prepared:
  - ▶ “Open and run”, or
  - ▶ Try to adjust some settings to get an even better force field
- ▶ **Deadline:** 1 July 2022
- ▶ <https://www.scm.com/news/params-reaxff-parametrization-challenge/>

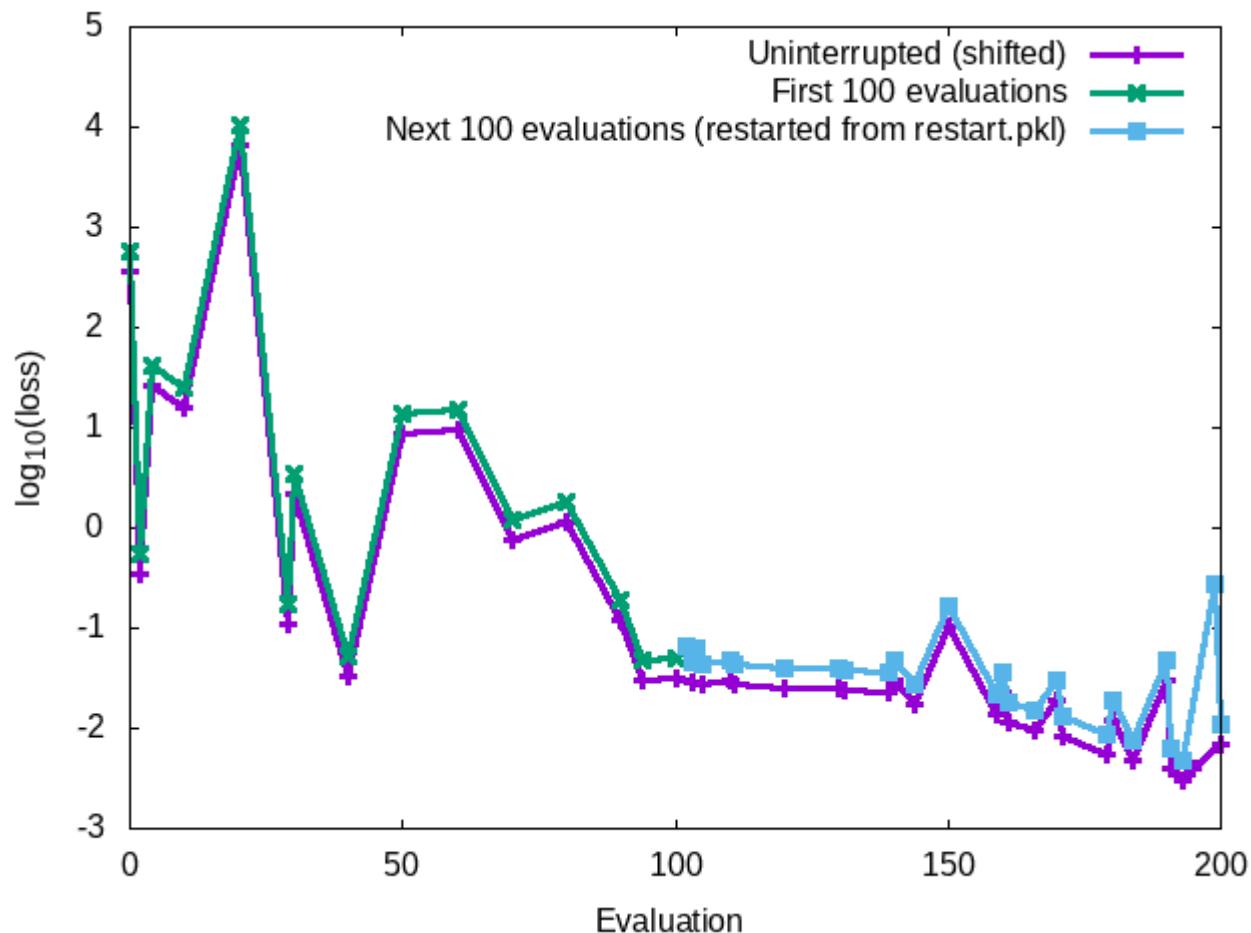


# 12 bonus features

## #1: Validation sets



## #2: Restart (continue) an optimization



## #3: The *params* Python library



```
ri.add_singlejob(water_ams_results_file,           # path to ams.rkf
                 properties={
                     'distance(0,1)': { # extract O-H bond Length
                         'weight': 2.0,
                         'sigma': 0.1,
                     },
                     'angle(1,0,2)': {}, # H-O-H angle, use default weight and sigma
                 },
                 task='GeometryOptimization',    # set task to GeometryOptimization
                 name='water_geo_opt')         # set a custom name
```

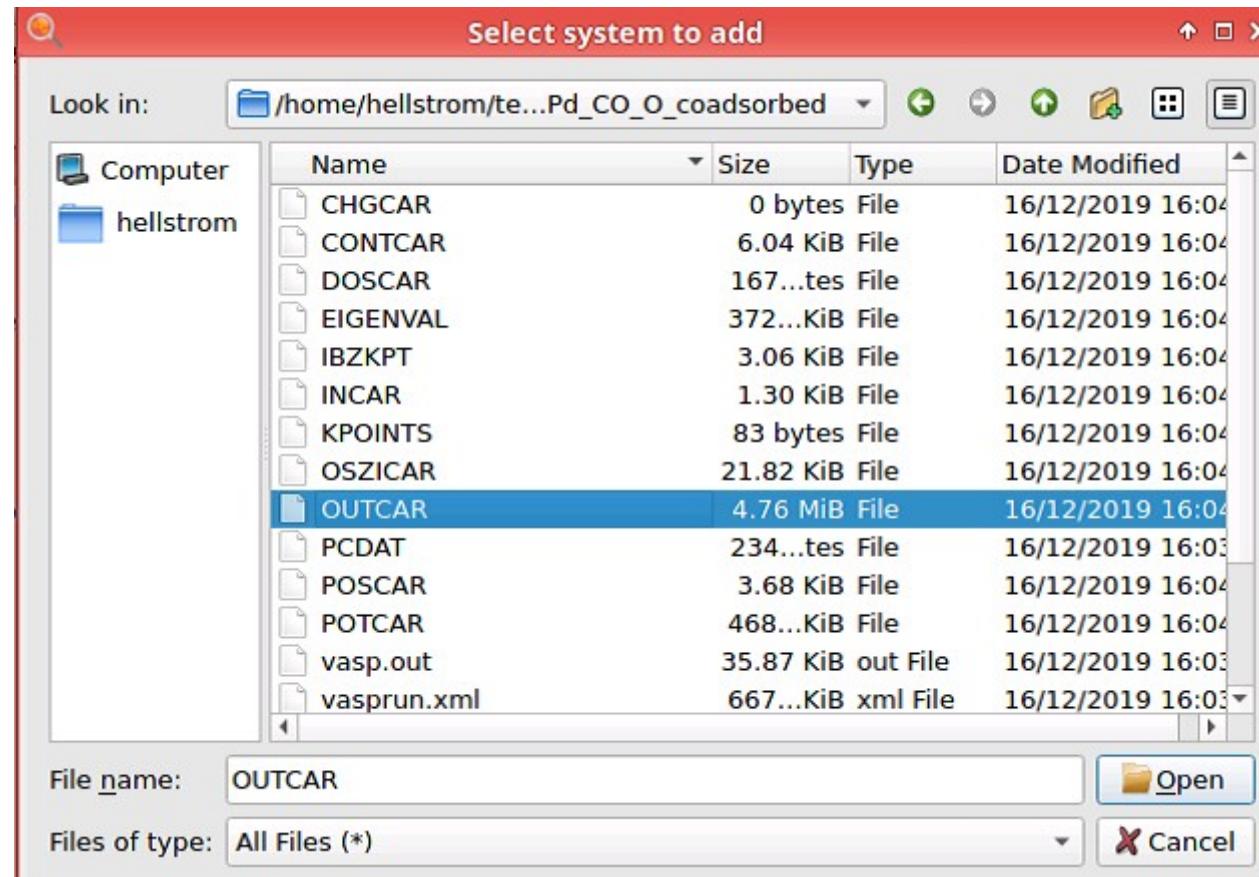
## #4: Experimental reference data

Energy:	+1.0*energy("LiF_bulk")-1.0*energy("Li_bulk")-0.5*energy("F2")
Sigma:	0.05442279126360184
Weight:	1.0
Unit:	eV
Values:	- 6.394

Use tab-completion after a " to cycle through matching JobIDs. Typing a " finishes the tab-completion.

Balance

## #5: Import VASP or Quantum ESPRESSO calculations



# #6: 14 GUI and Python tutorials

## ▼ 2. Tutorials

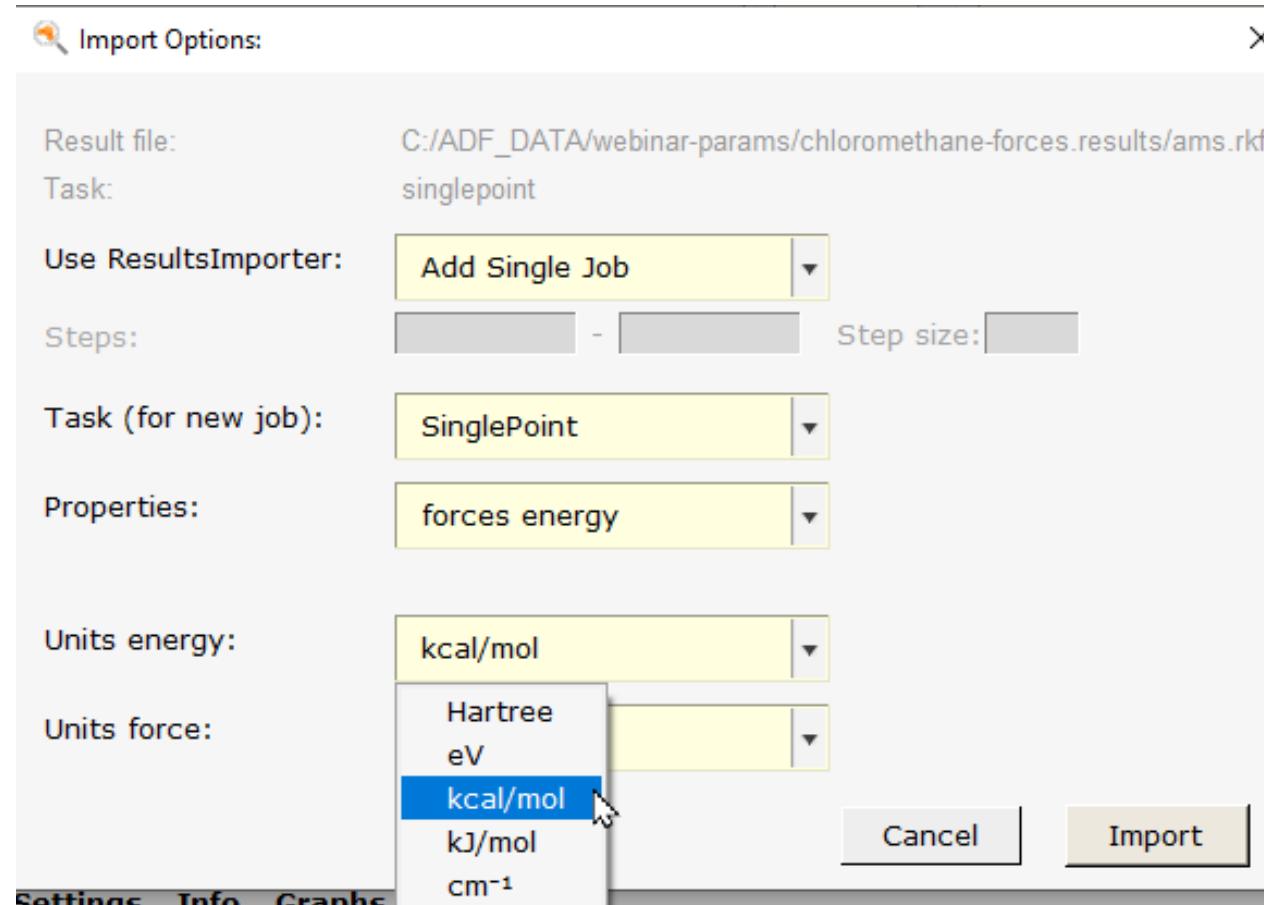
- 2.1. Introduction to parametrization
- 2.2. Getting Started: Lennard-Jones Potential for Argon
- 2.3. Import training data (GUI)
- 2.4. Import training data (Python)
- 2.5. ReaxFF: Gaseous H<sub>2</sub>O
- 2.6. ReaxFF: Adsorption on ZnS(110)
- 2.7. ReaxFF: Convert old training sets to ParAMS format
- 2.8. ReaxFF: Training set for cobalt
- 2.9. GFN1-xTB: Lithium fluoride
- 2.10. Training and validation sets
- 2.11. Restarting (continuing) an optimization
- 2.12. Calculate reference values with ParAMS
- 2.13. The params Python library
- 2.14. DFTB repulsive potential

- 2.2. Getting Started: Lennard-Jones Potential for Argon

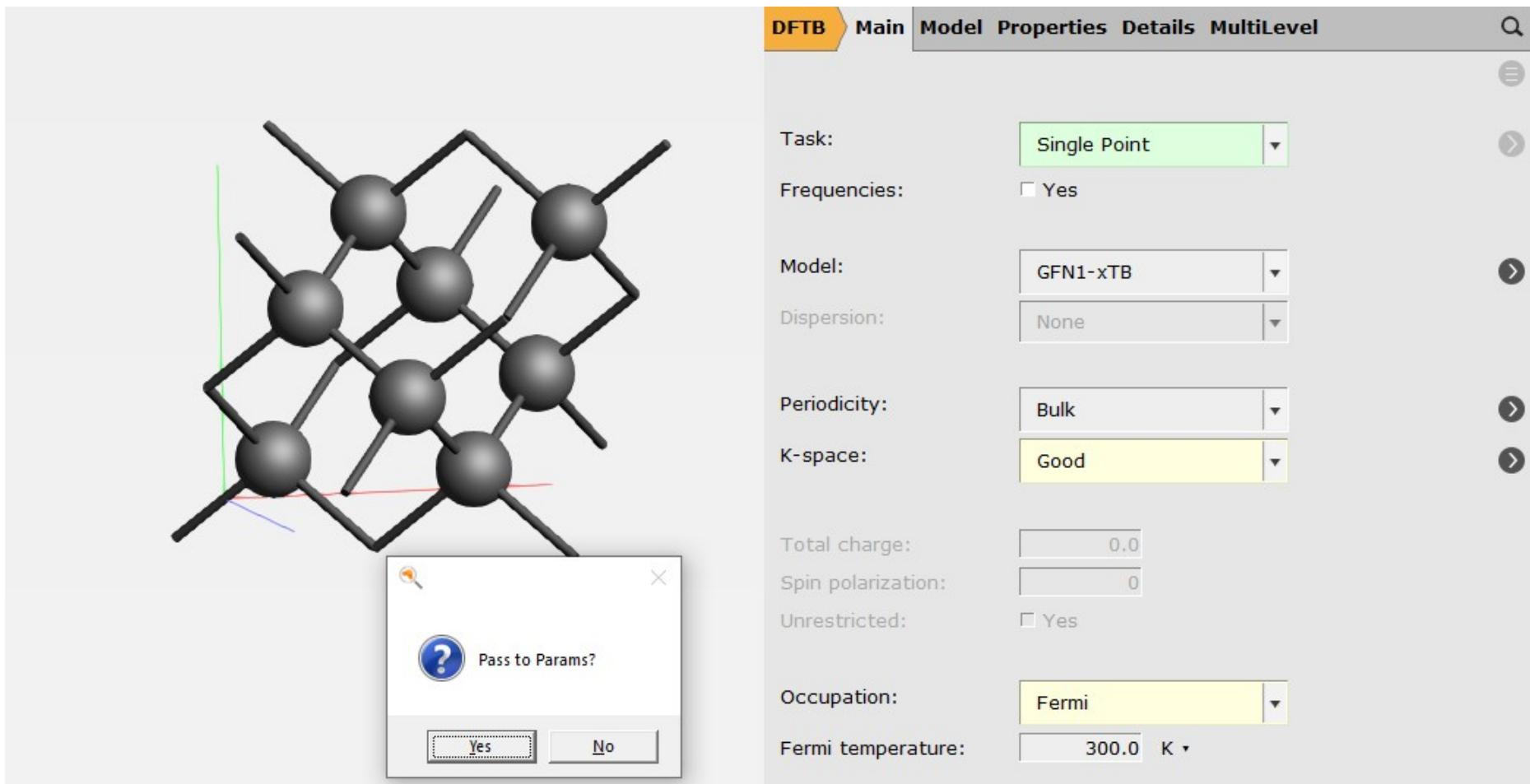
- 2.2.1. Lennard-Jones Parameters, Engine, and Interface
- 2.2.2. Files
- 2.2.3. ParAMS input
  - 2.2.3.1. Parameter interface (parameter\_interface.yaml)
  - 2.2.3.2. Job Collection (job\_collection.yaml)
  - 2.2.3.3. Training Set (training\_set.yaml)
  - 2.2.3.4. ParAMS settings (params.conf.py)
- 2.2.4. Run the example
- 2.2.5. Parametrization results
  - 2.2.5.1. The best parameter values
  - 2.2.5.2. Correlation plots
  - 2.2.5.3. Error plots
  - 2.2.5.4. Parameter plots
  - 2.2.5.5. Editing and Saving Plots
  - 2.2.5.6. Predicted values
  - 2.2.5.7. Loss contributions
  - 2.2.5.8. Summary statistics
  - 2.2.5.9. All output files

<https://www.scm.com/doc/params/examples/examples.html>

## #7: Work in your preferred units



## #8: Modify job settings with AMSinput



The screenshot shows the AMSinput software interface. On the left, a 3D visualization of a crystal lattice structure is displayed, consisting of dark grey spheres connected by black lines. A small pop-up window titled "Pass to Params?" with a question mark icon contains two buttons: "Yes" and "No". The main interface has a top navigation bar with tabs: DFTB (highlighted in yellow), Main, Model, Properties, Details, and MultiLevel. Below the navigation bar, the "Main" tab is active. The job settings are listed on the right:

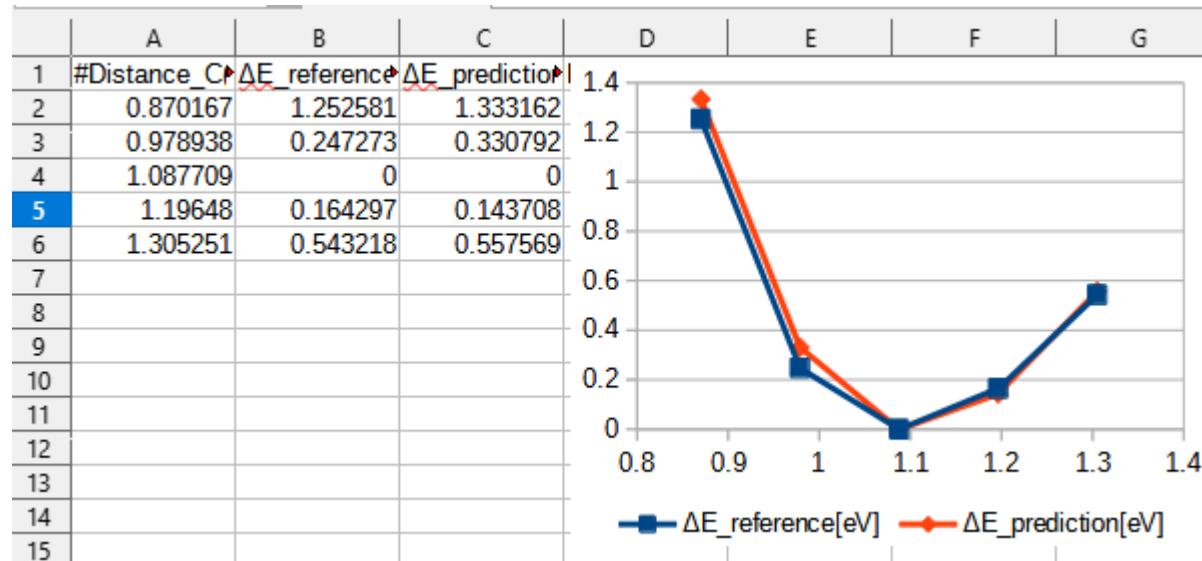
- Task:** Single Point
- Frequencies:**  Yes
- Model:** GFN1-xTB
- Dispersion:** None
- Periodicity:** Bulk
- K-space:** Good
- Total charge:** 0.0
- Spin polarization:** 0
- Unrestricted:**  Yes
- Occupation:** Fermi
- Fermi temperature:** 300.0 K

## #9: Human-readable input in .yaml format

```
---
  dtype: DataSet
  version: '2022.101'
---
  Expression: charges('water_singlepoint')
  Weight: 1.0
  Sigma: 0.1
  ReferenceValue: |
    array([-0.83399999,  0.417       ,  0.417       ])
  Unit: au, 1.0
---
  Expression: forces('water_singlepoint')
  Weight: 1.0
  Sigma: 3.557463138142747
  ReferenceValue: |
    array([[ 0.25021751, -0.01895832, -0.        ],
           [-0.03370832, -0.12831032, -0.        ],
           [-0.21650919,  0.14726863, -0.        ]])
  Unit: kcal/mol/angstrom, 1185.8210460475823
...
```

## #10: Human-readable output: import directly to Excel, gnuplot, ...

```
#Distance_C(1)--H(5) [angstrom] ΔE_reference[eV] ΔE_prediction[eV] E_reference[eV]
0.870167 1.252581 1.333162 -53.399365
0.978938 0.247273 0.330792 -54.404673
1.087709 0.000000 0.000000 -54.651946
1.196480 0.164297 0.143708 -54.487649
1.305251 0.543218 0.557569 -54.108729
```



# #11: Convert from old ReaxFF training set format (<AMS2022) to ParAMS



Old File	+	(Optional File)	=	New File
geo		control		job_collection.yaml
trainset.in				training_set.yaml
ffield		params		parameter_interface.yaml

cripting > scm > params > examples > import\_old\_ReaxFF > polymer

The screenshot shows a file explorer interface with a navigation bar at the top. The current path is 'cripting > scm > params > examples > import\_old\_ReaxFF > polymer'. Below the path is a search bar with a magnifying glass icon and the word 'Search'. The main area displays a list of files:

Name	Date modified	Type	Size
ffield	28/01/2022 11:25	File	27 KB
geo	28/01/2022 11:25	File	508 KB
params	28/01/2022 11:25	File	5 KB
README.txt	28/01/2022 11:25	Text Document	1 KB
trainset.in	28/01/2022 11:25	IN File	22 KB

## #12: Recalculate a trajectory with a different method



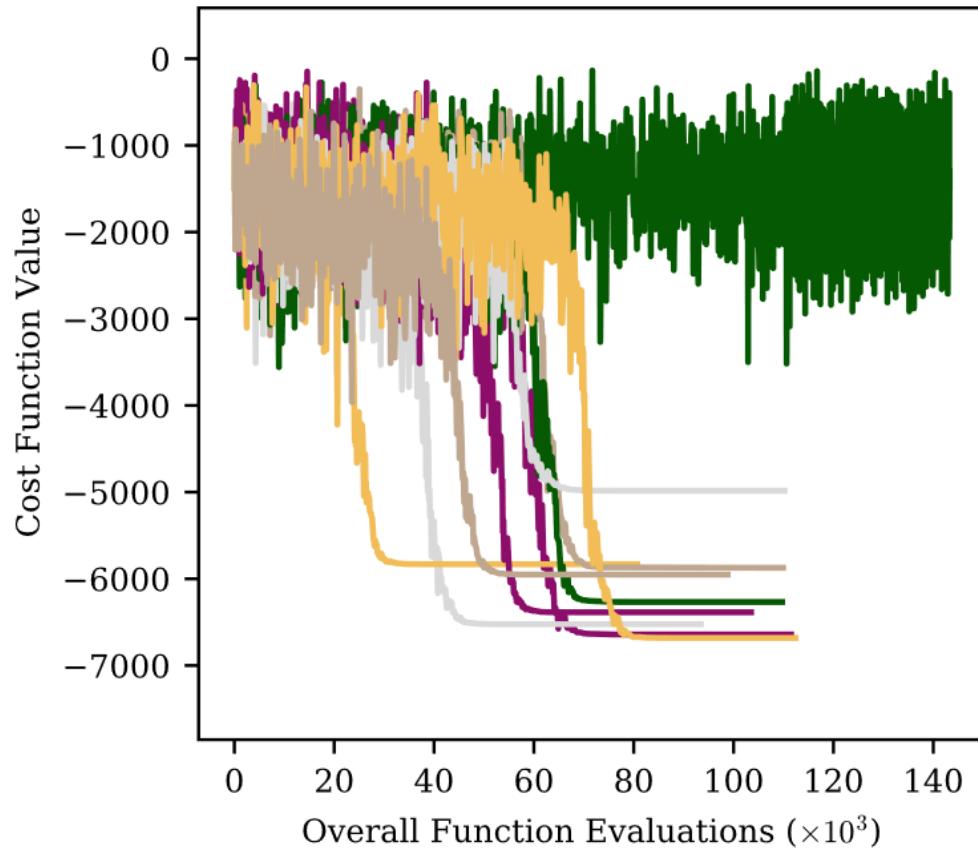
- ▶ Recalculate all or some frames from molecular dynamics, PES scans, ...
- ▶ Compare results or import as reference data into ParAMS

The screenshot shows the ParAMS software interface with the following details:

- Top Navigation Bar:** ADF (highlighted in yellow), Main, Model, Properties, Details, MultiLevel, Search icon.
- Section Title:** Replay
- Restart from:** -params/2-ether-cont.NPT.results/ams.rkf
- Frames:** 100 200 300
- Store all result files:**  Yes

# Future developments: AMS2023?

- ▶ Improvements to the input
- ▶ Improvements to the graphical user interface
- ▶ Run multiple optimizations at the same time with GloMPO



# Summary

- ▶ ParAMS and AMS make it easy to create and validate
  - ▶ ReaxFF force fields
  - ▶ DFTB (actually GFN1-xTB) parameters
- ▶ Train to reaction energies, forces, charges, bond scans, ...
- ▶ Results shown in many different graphs and tables
  - ▶ Updated on-the-fly, even on a remote machine!
- ▶ Use AMS to address your research problems
- ▶ Participate in the ParAMS challenge!

