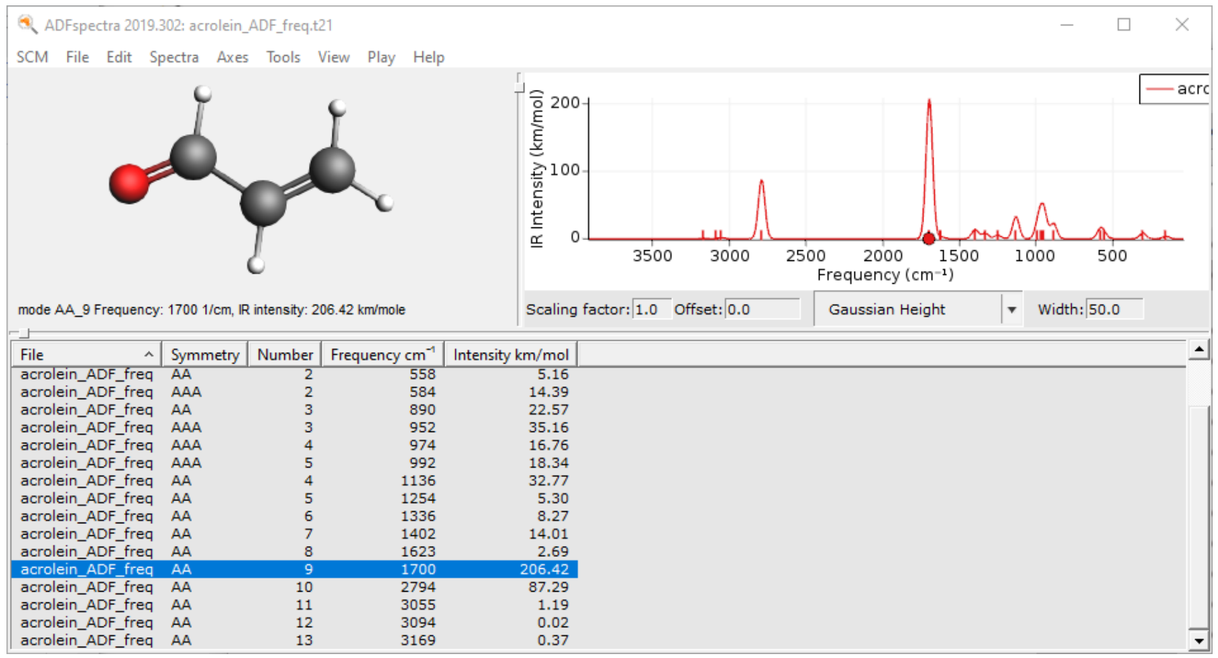
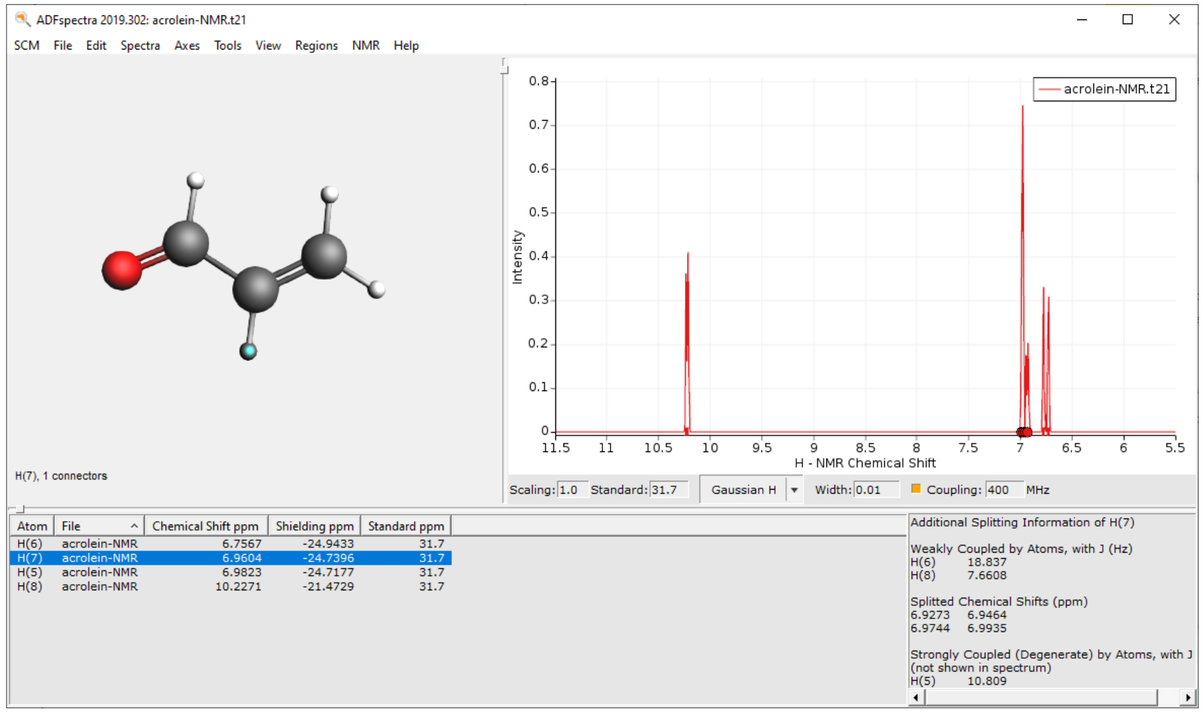
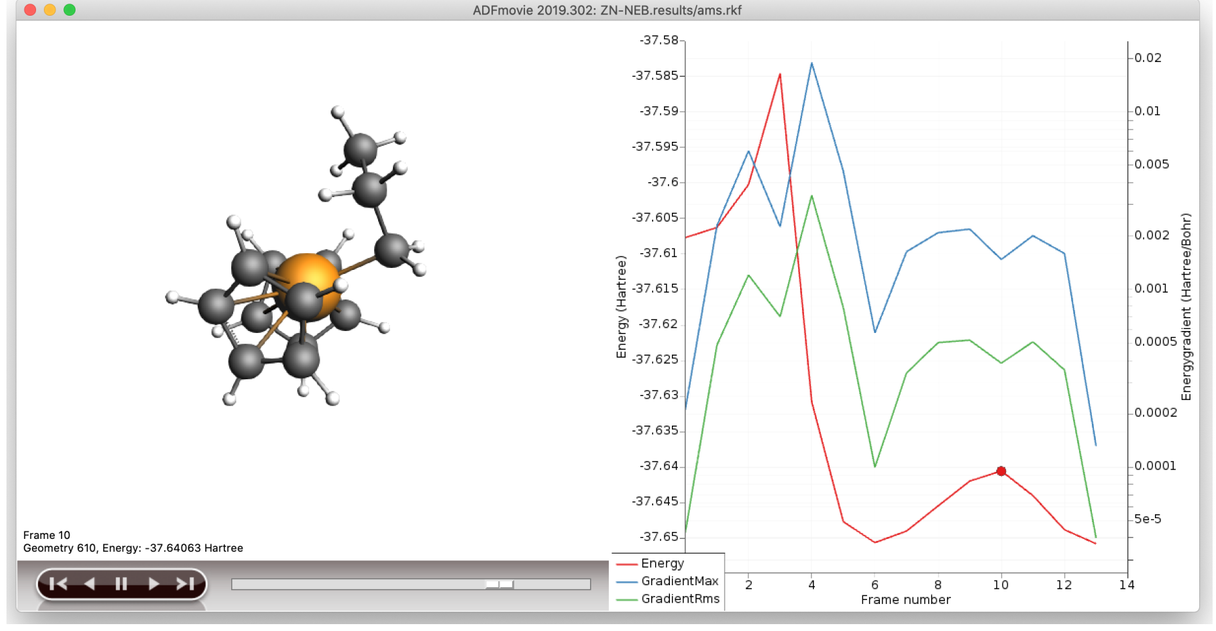
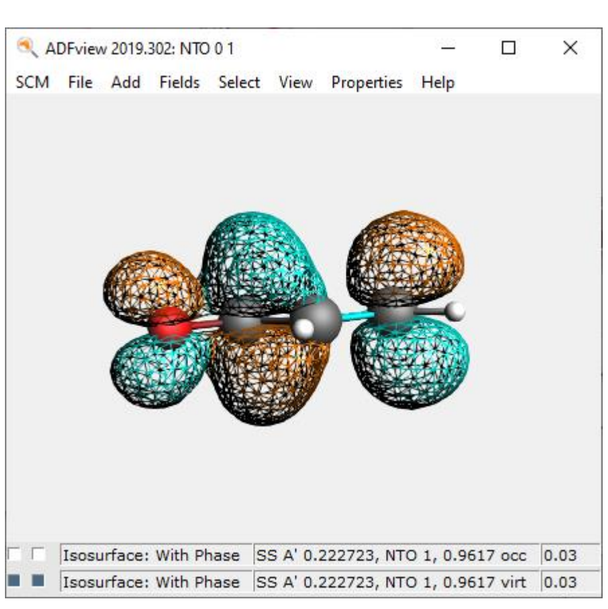
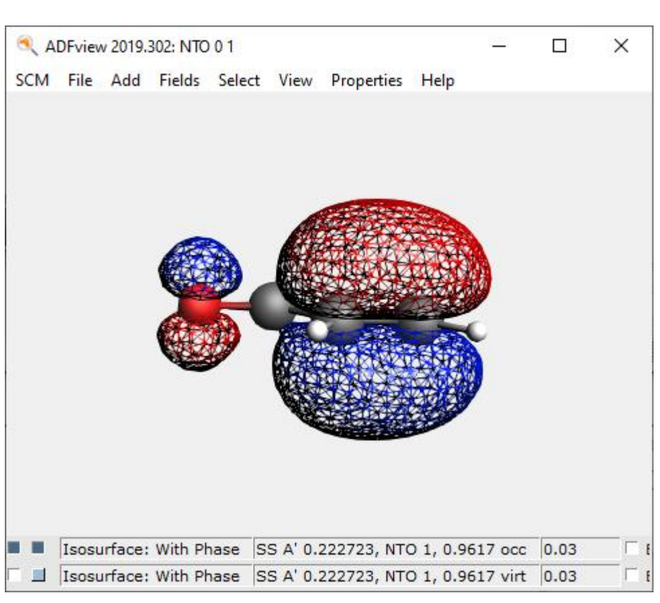
Getting started with AMS!











SCM
Software for Chemistry & Materials

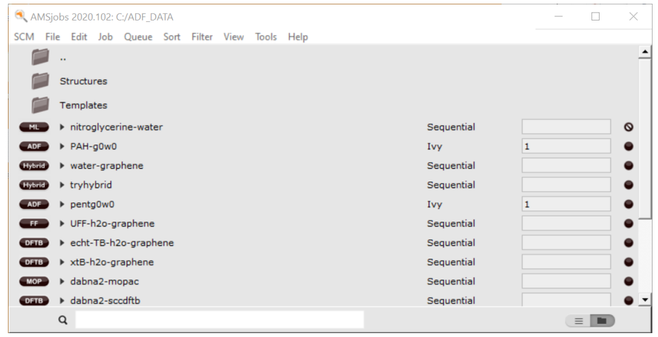
Getting started with the GUI, TU Delft, 21 January 2021

SCM support: support@scm.com

Getting started with the GUI

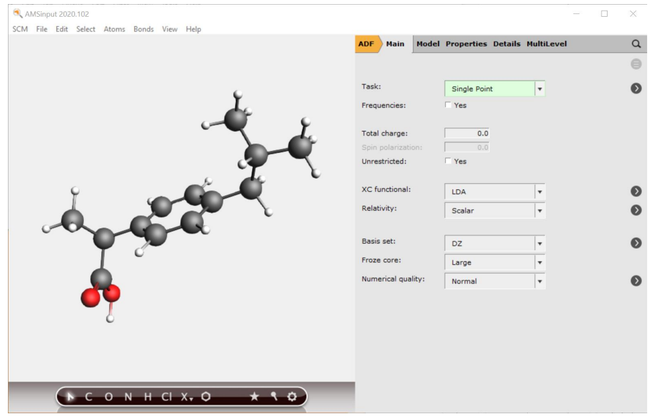
Starting AMSjobs: job bookkeeping

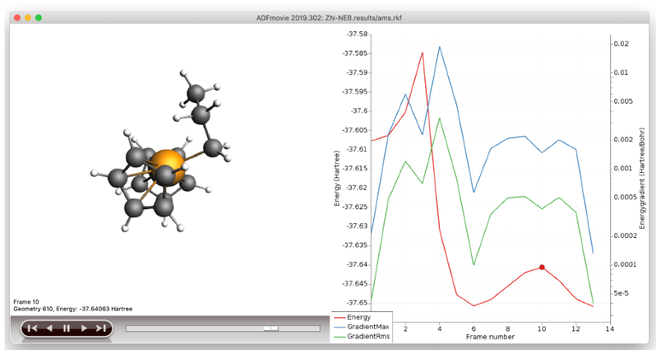
- Win: dbl-click desktop item
- Mac: open Application
- Linux: run $AMSBIN/adfjobs

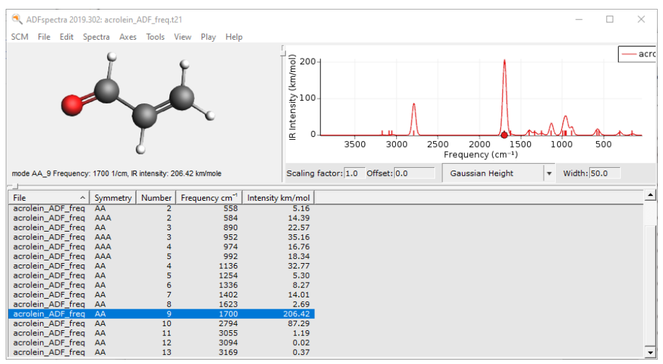


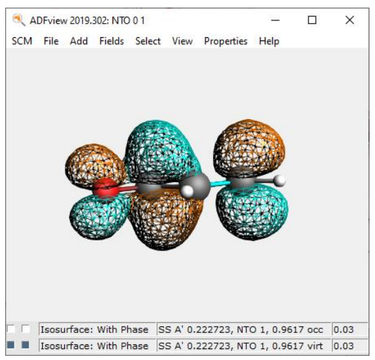
- AMSInput: define system + properties + settings

- Other: (View, Levels, Movie, Spectra, Band Structure, AMSTrain, Microkinetics, COSMO-RS, KF Browser…)
  - Open from result file, SCM menu or e.g. by dbl-clicking ‘amsinput.exe’ (Win) or running ‘$AMSBIN/amsinput’

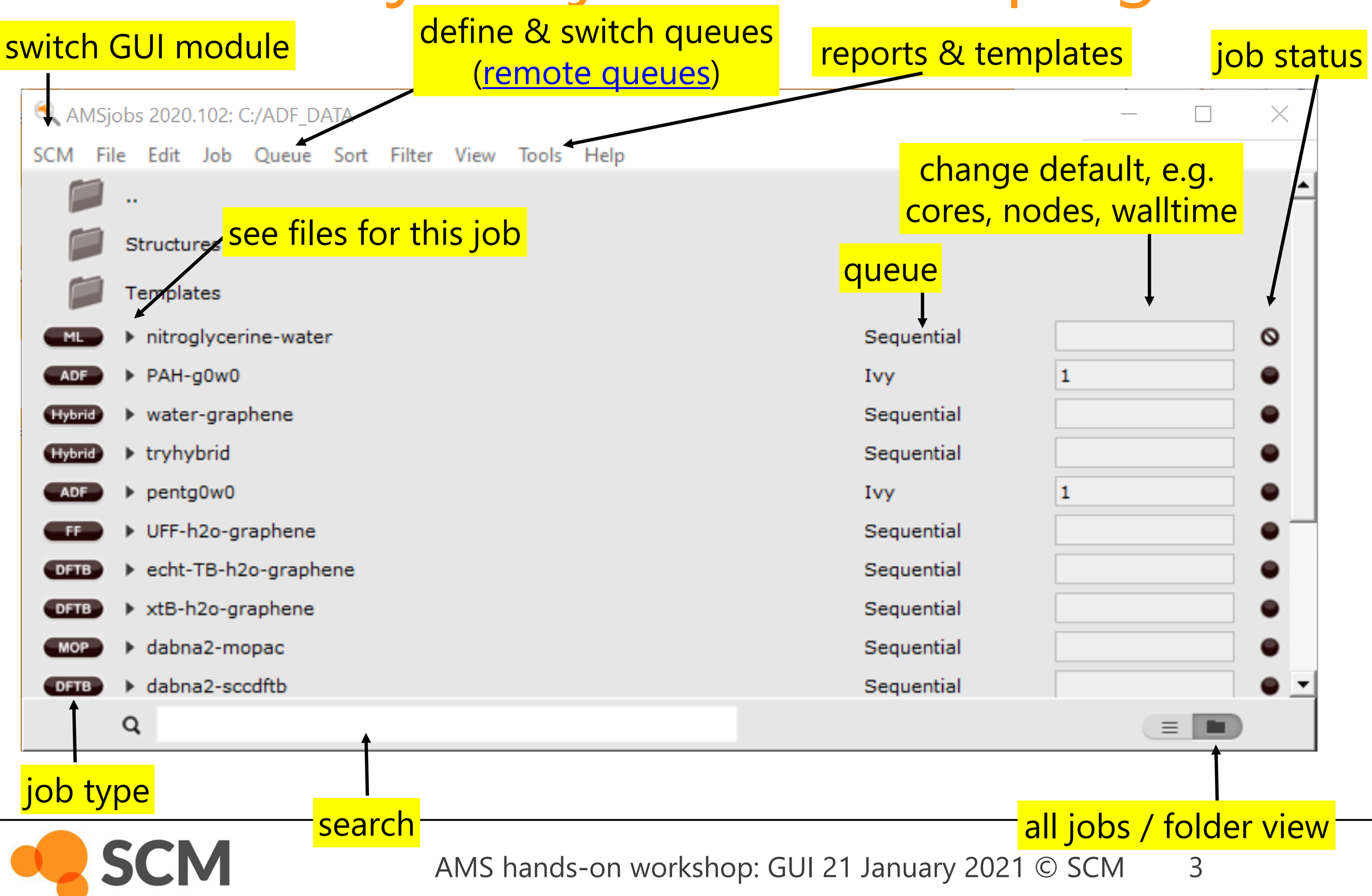




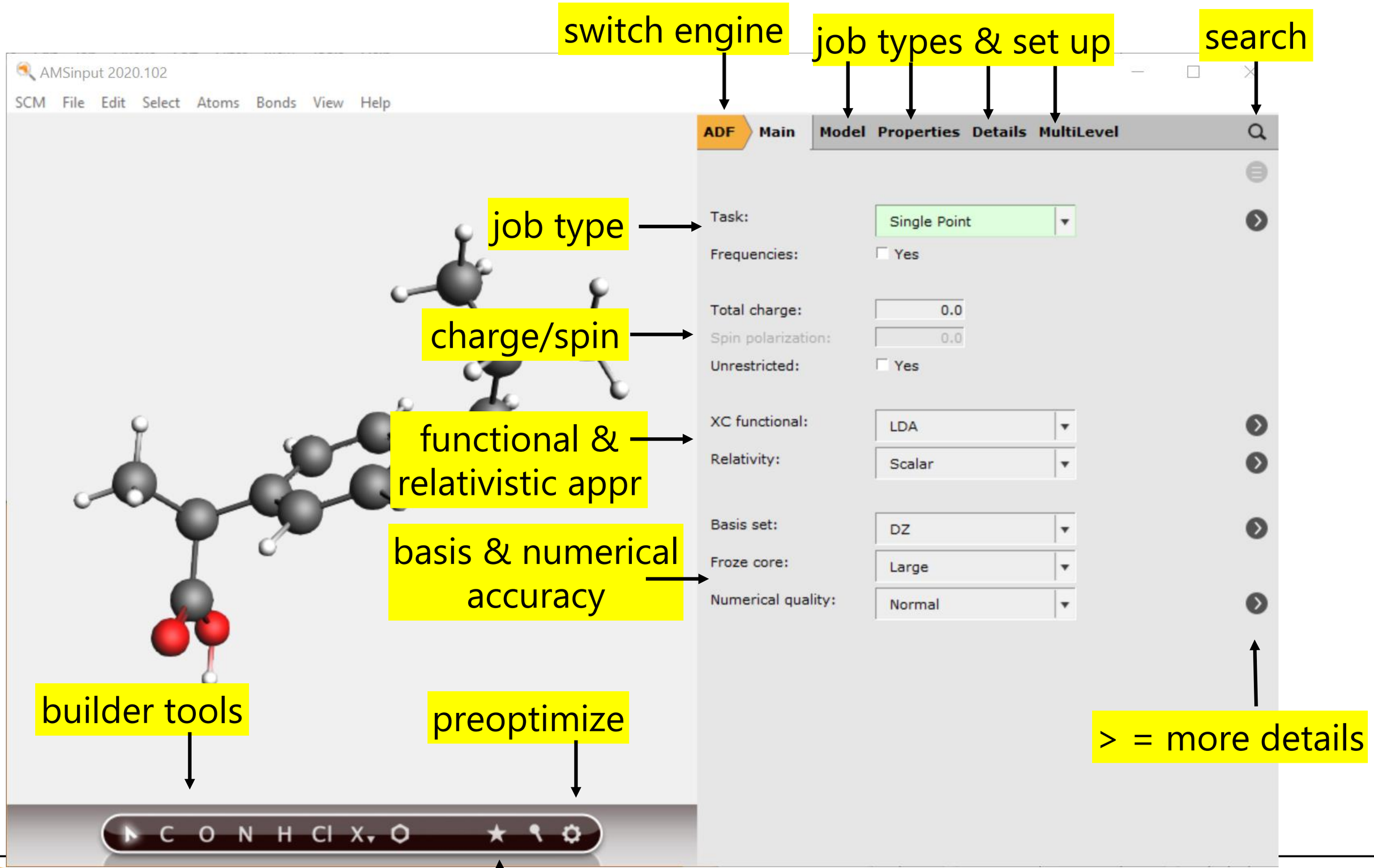




AMSjobs: job bookkeeping



Basic calculations & settings



GUI input 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**

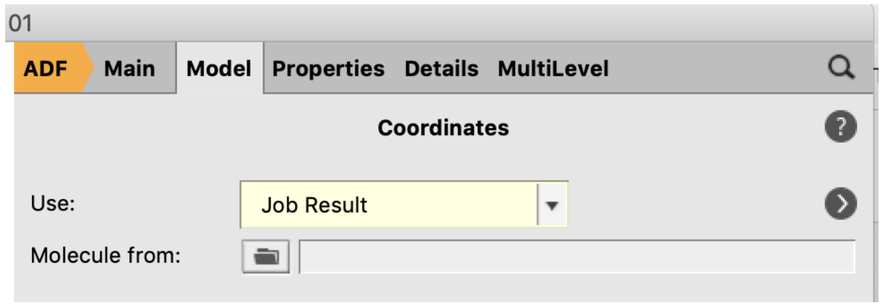
GUI input editor controls

- 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**

Using the GUI more efficiently

1. Chained jobs
   - Model -> coordinates use Job results
   - E.g. first do pre / partial optimization
   - Can not be used to also read in Hessian
     - Python scripting could work (do check on nimag e.g.)



2. Preset
   - If you always use same XC, basis set, relativity & quality, etc. you can save it:
     - File -> Save as preset (all fields different from default)
     - File -> Save as full preset (all input options)
   - Load this: File -> Preset -> 'Your preset' on future jobs with the same setting

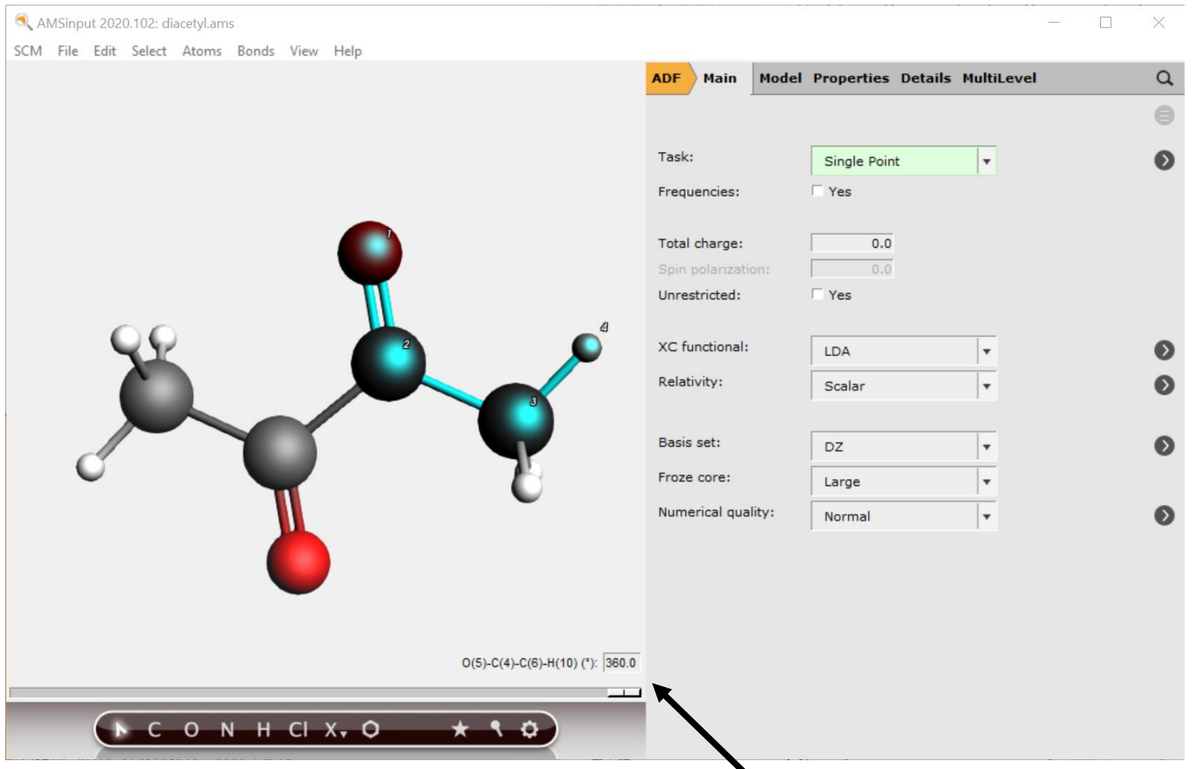
3. AMSprepare (& report)
   - In amsjobs select a job, tools -> prepare
   - Now you can run the same job but with different settings (e.g. basis set, xc, …)
   - With adfreport you can build a report to visualize results (e.g. distances)
   - (also consider Python scripting with PLAMS)

Building molecules (tutorials)

- Search molecules in GUI
- Import: InChI, SMILES, xyz, cif, pdb, …

- Included structure library + building

- **Excercise:** Build diacetyl ($C_4H_6O_2$)
  - By searching for it in the GUI
  - By starting from the builder tools
    use ‘2’ for double bonds, Ctrl+E adds H’s
  - By importing SMILES (e.g. from Wikipedia)
  - Select multiple atoms to change bond, angle, dihedral



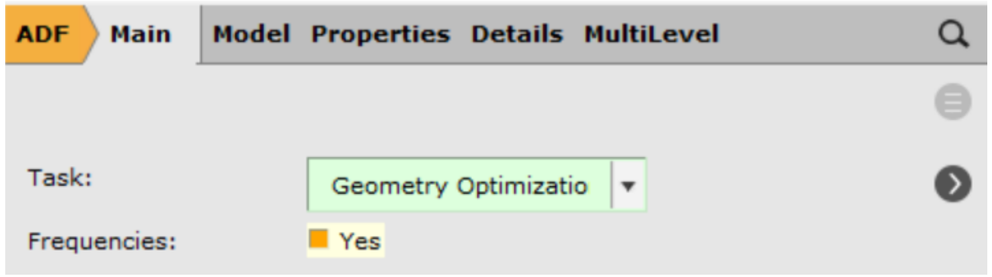
slide or type value

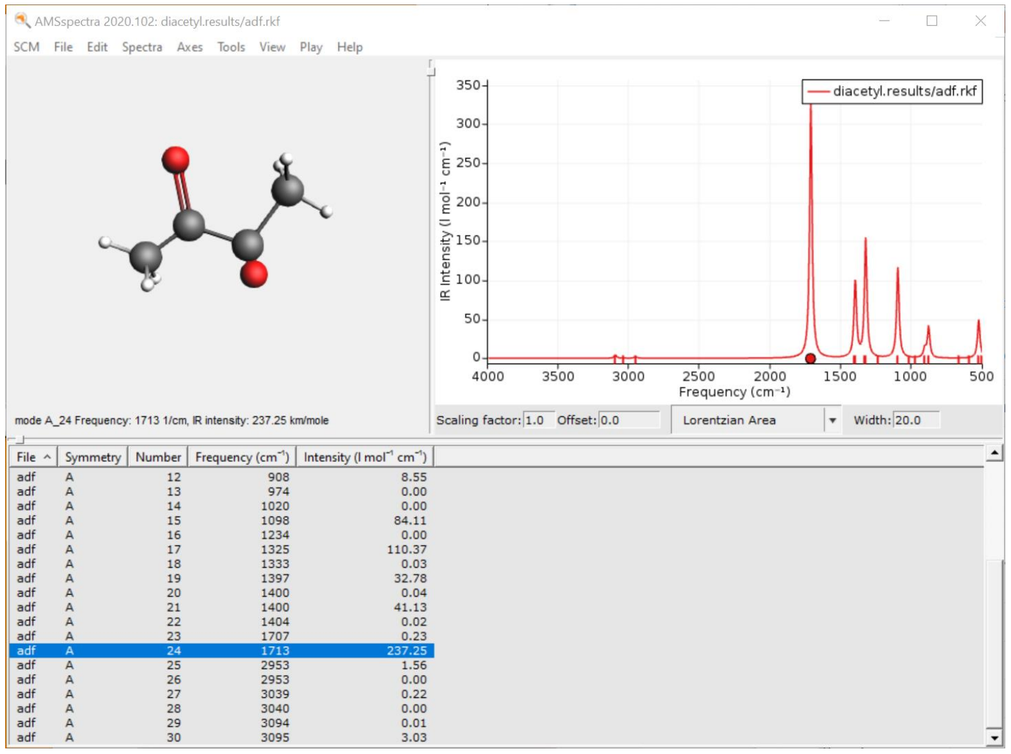
- Symmetrize (C_{2h}), pre-optimize (UFF, MOPAC, DFTB, MLPotential)

- Think about conformers!

Spectra: IR, other vibrational

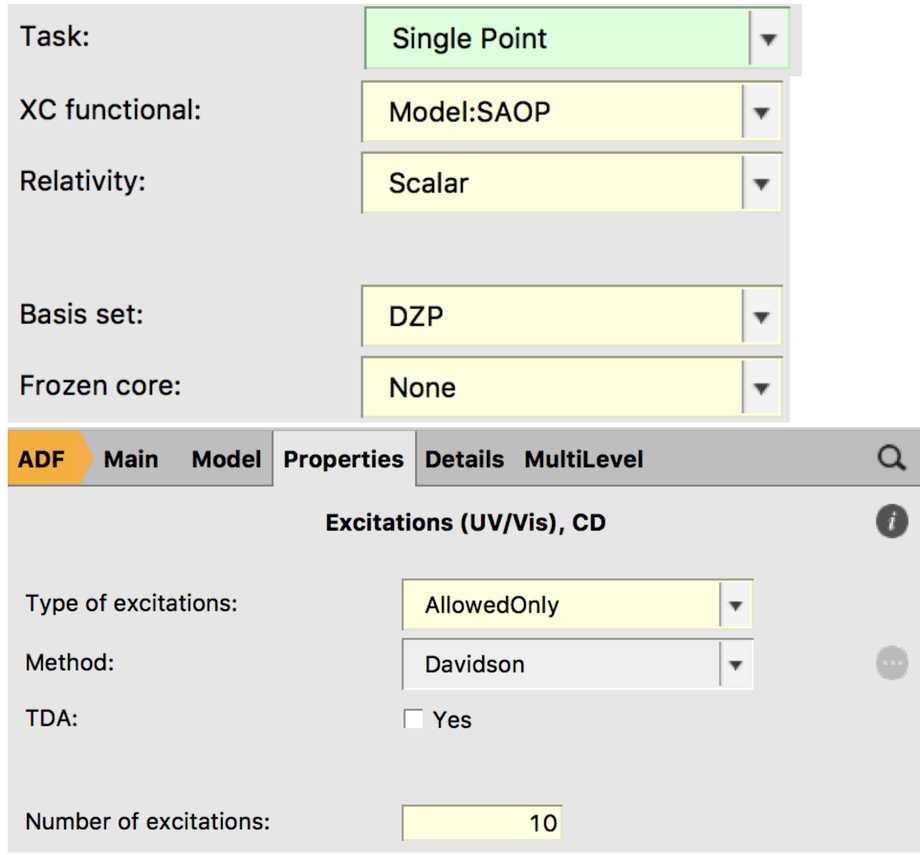
- **Excercise:** Calculate & visualize frequencies
  - Optimize geometry at same level as frequency calc.
  - Task = Geometry Opt + Frequencies = Yes
  - Try a few different methods:
    - ADF: PBE-D4/DZP
    - DFTB: DFTB3-D3-BJ/3ob-3-1
    - MOPAC
  - Visualize: AMSSpectra, animate some modes
  - Axes-> Molar Absorption Coefficient
  - Tweak broadening
  - Compare to NIST
  - Play with Spectra-> PVDOS





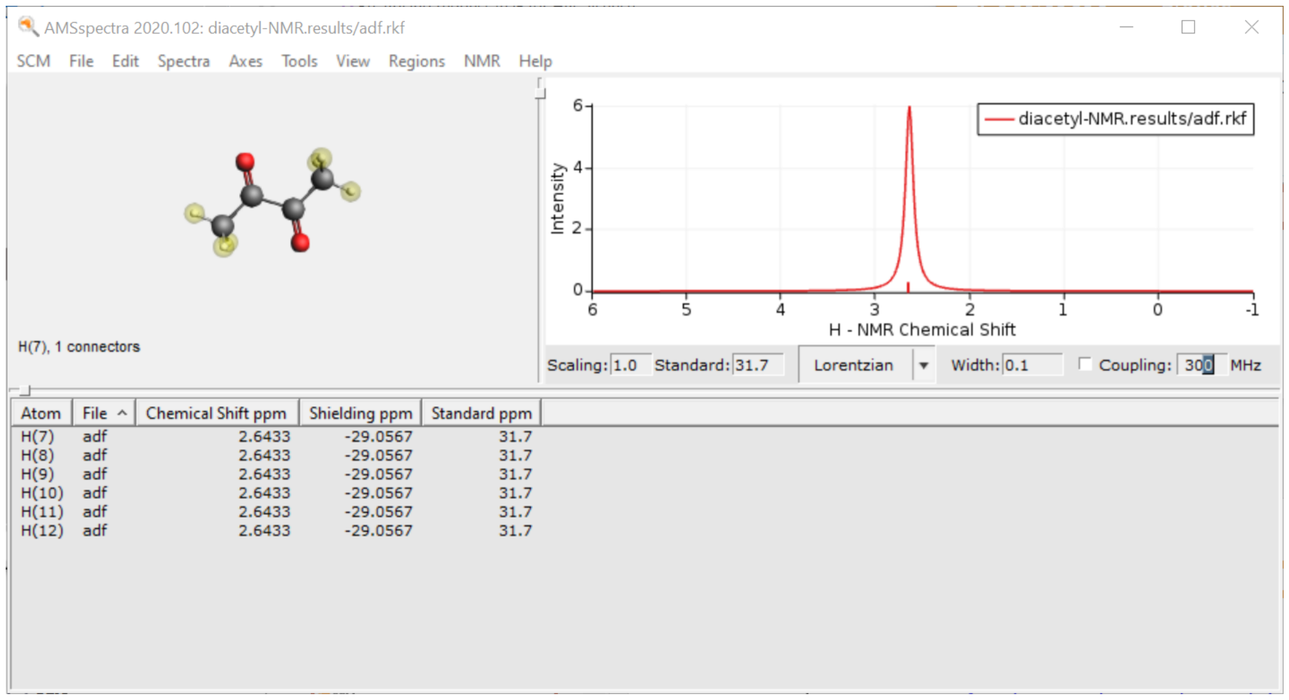
Spectra: UV/VIS

- Exercise:
  - With ADF: calculate 10 allowed excitations
    - use SAOP model potential, DZP (or TZP), no core
    - See also UV/VIS FAQ for tips
  - Go to spectra, change x-axis to nm
  - Increase the line width to ~10
  - Visualize the pi-pi* NTOs at ~205nm (click on NTO1)
  - Visualize the MOs strongest Single Orbital Transition
  - Compare to NIST data which peaks are missing?
    - Forbidden transitions? Spin-orbit coupling? Vibronic?
    - Check out
  - More exercises
    - Rerun with method ‘sTDA’ and tick TDA
    - Also try TD-DFT+TB (ADF)
    - and TDDFTB (DFTB3/3ob-3-1, GFN-xTB)
    - (can use the same PBE-D4 optimized geometry)



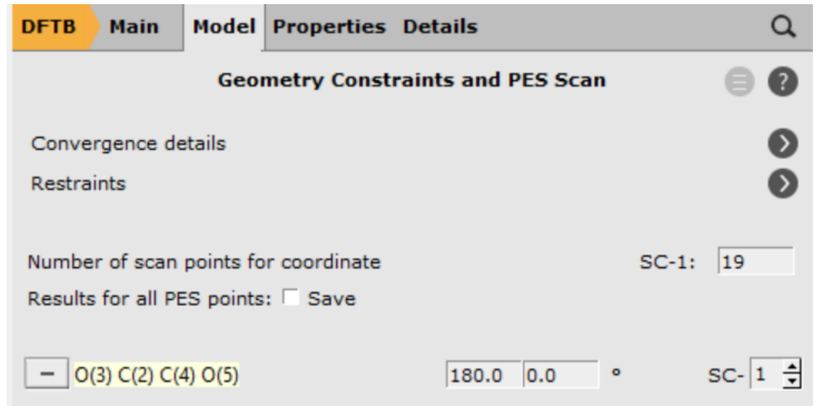
Spectra: NMR

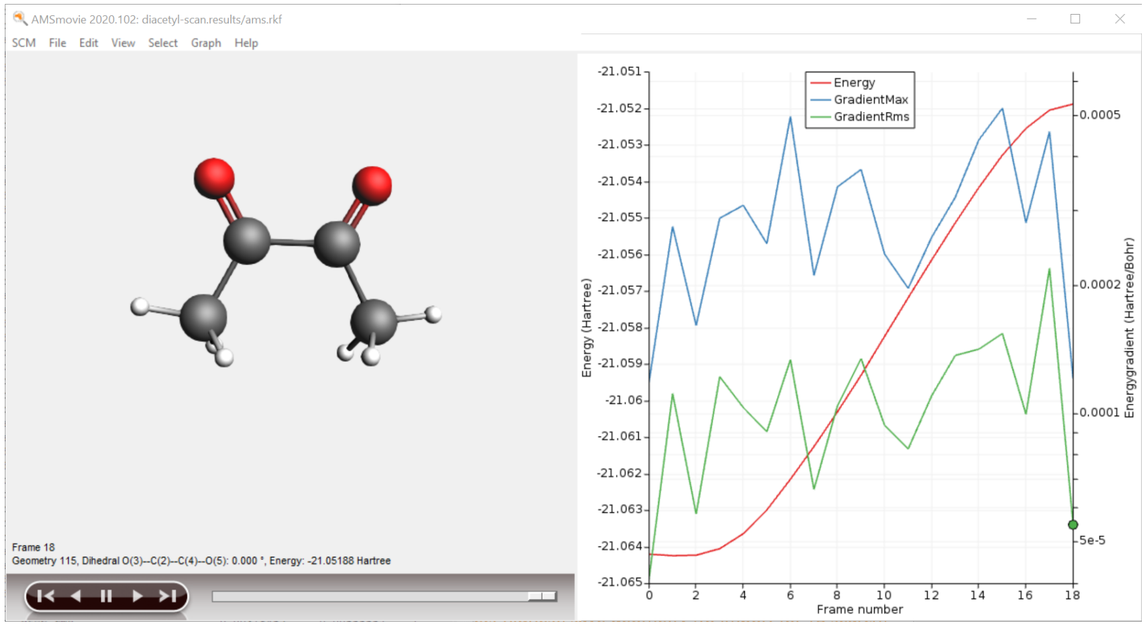
- Exercise:
  - See also NMR FAQ for tips + advanced tutorials
  - Use PBE0 + TZP, Scalar, no core
  - Select Properties -> NMR
    - select shielding for all H
  - Spectrum, NMR-> Chem. Equivalent regions
    - Note all H are equivalent (rotation), no coupling
  - Note the internal ref. uses different settings!
    - Recalculate TMS with same set up



PES: conformers, scan dihedral

- Exercises:
  - Switch the engine to Conformers, run, visualize -> AMSMovie
    - Does it find all conformers :) ? Maybe try a larger molecule?
    - Switch to, e.g. DFTB, and from Model -> Coordinates, Use: Selected File, select your.sdf
    - Do a frequency run on all geometries and visualize a Boltzmann-averaged spectrum
  - Take a DFTB input, set task to PES Scan, click >
    - Select dihedral and scan in 19 points from 180-0
    - Wait for calculation to finish -> AMSMovie
    - One can save geometries to start TS search (see later)





Quick thermodynamic properties

- Exercise:
  - Open SCM -> COSMO-RS
  - In the SMILES input, put CC(=O)C(=O)C and Add
  - Properties -> Pure compound
  - Compare some properties (density, boiling point) (e.g. Wikipedia)

Property		Unit
Boiling point	346.746	K
Critical pressure	51.21	bar
Critical temperature	524.603	K
Critical volume	0.195	L/mol
Liquid density	0.816	kg/L
Dielectric constant	10.985	
Absolute entropy (ideal gas)	309.848	J/(mol K)
Flash point	270.523	K
Gibbs energy of formation (ideal gas)	-111.468	kJ/mol
Net enthalpy of combustion	-1652.692	kJ/mol
Std. state enthalpy of formation	-188.906	kJ/mol
Enthalpy of fusion	17.129	kJ/mol
Enthalpy of formation (ideal gas)	-157.71	kJ/mol
Enthalpy of sublimation	49.534	kJ/mol
Melting point	213.82	K
Liquid molar volume	0.069	L/mol
Parachor	161.085	
Solubility parameter	10.098	√(MPa)
Triple point temperature	213.778	K
Van der Waals area	91.576	$Å^2$
Van der Waals volume	63.229	$Å^3$