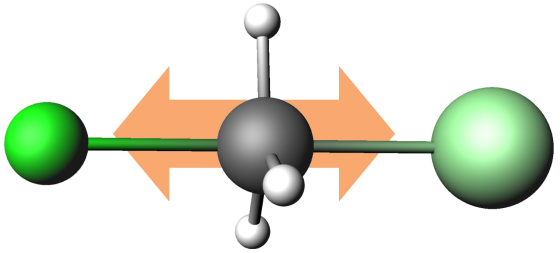
Transition States

- 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

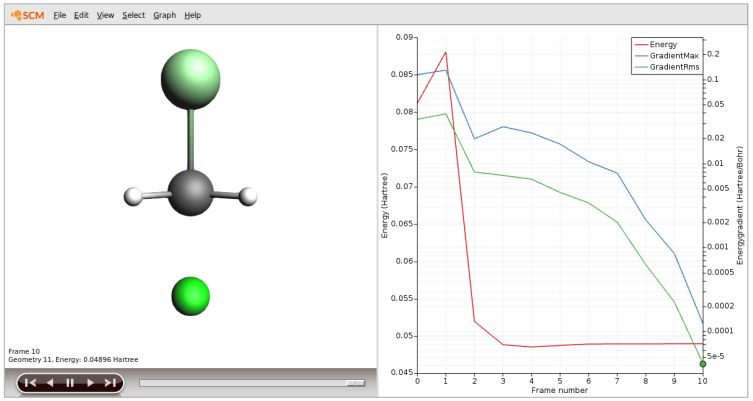
- In AMSinput: build Cl···CH_3···F guess (or import ClCH3F.xyz)



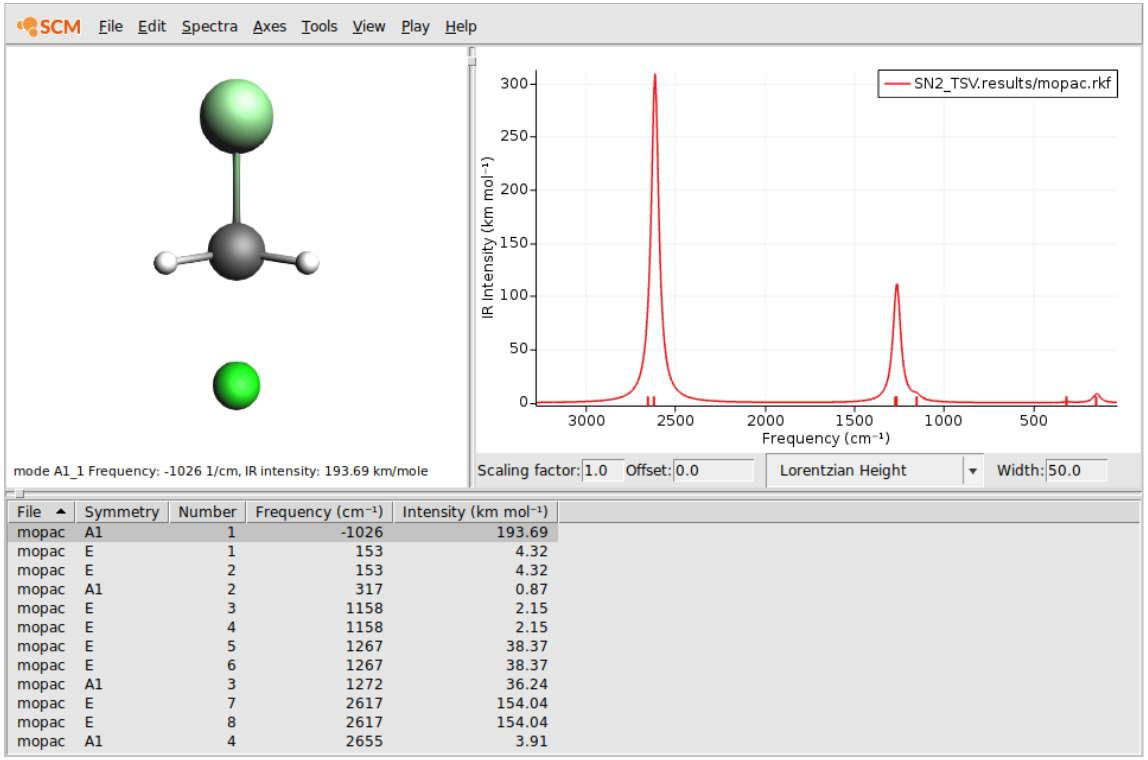
- Switch **ADF** → **Mopac**
  - **Task → Transition State**
    for larger systems ❯ to set details e.g. reaction coordinate
  - **Frequencies →** tick □ **Yes**
  - **Spin polarization → 1**
- Save and run job

SN2 Transition State Analysis

- SCM → Movie
  to inspect transition state search



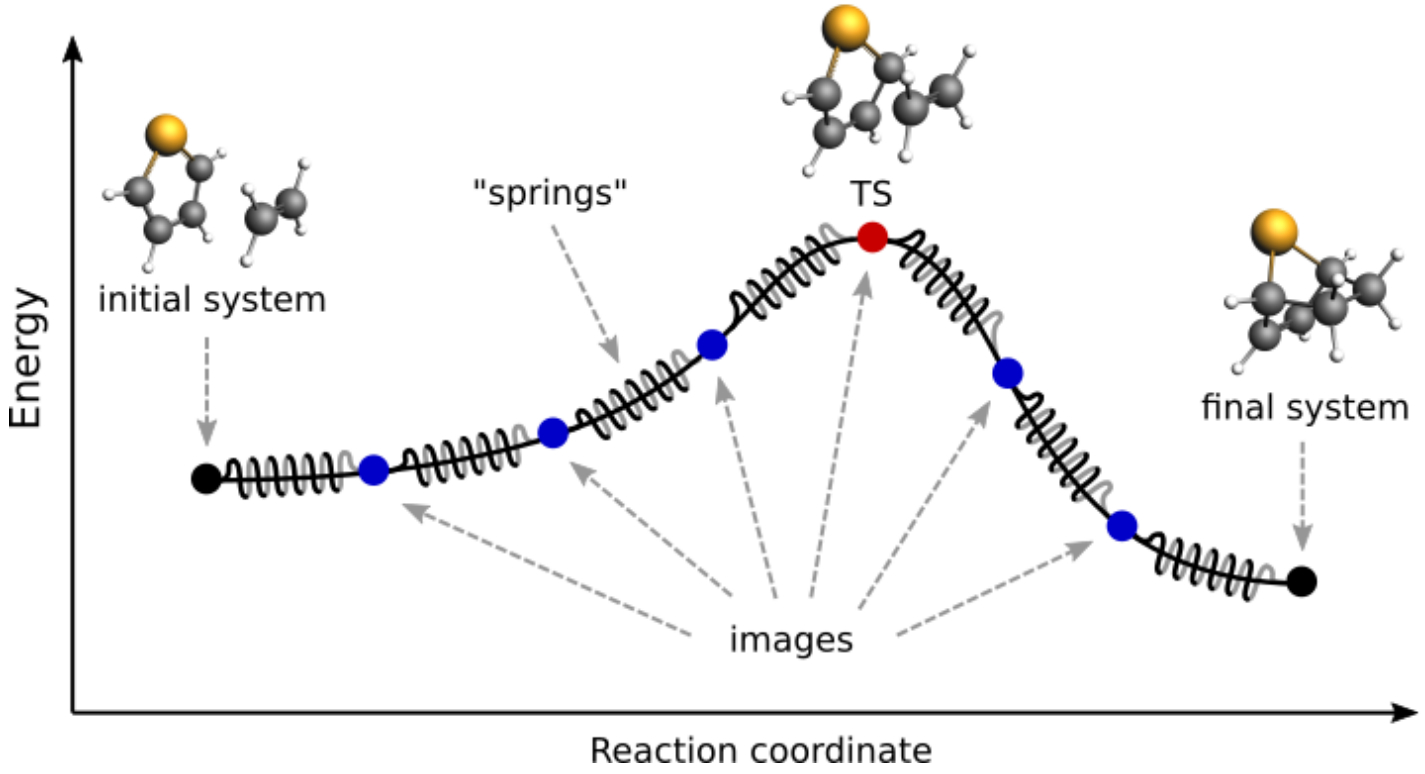
- SCM → Spectra
  to analyze reaction mode
  - *One* negative frequency
  - Click on negative mode
    to see movie of motion



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

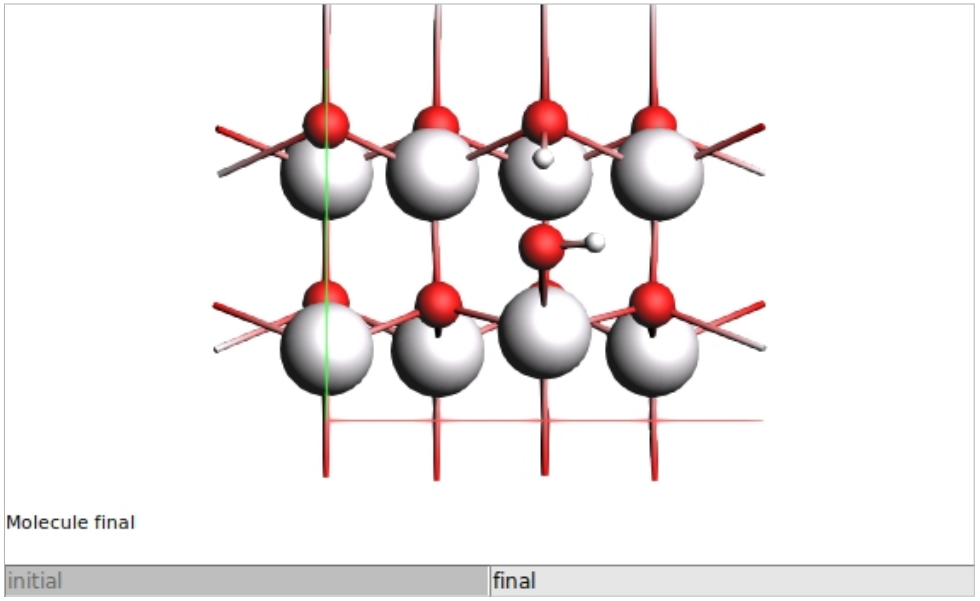
Nudged Elastic Band (NEB)

- 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

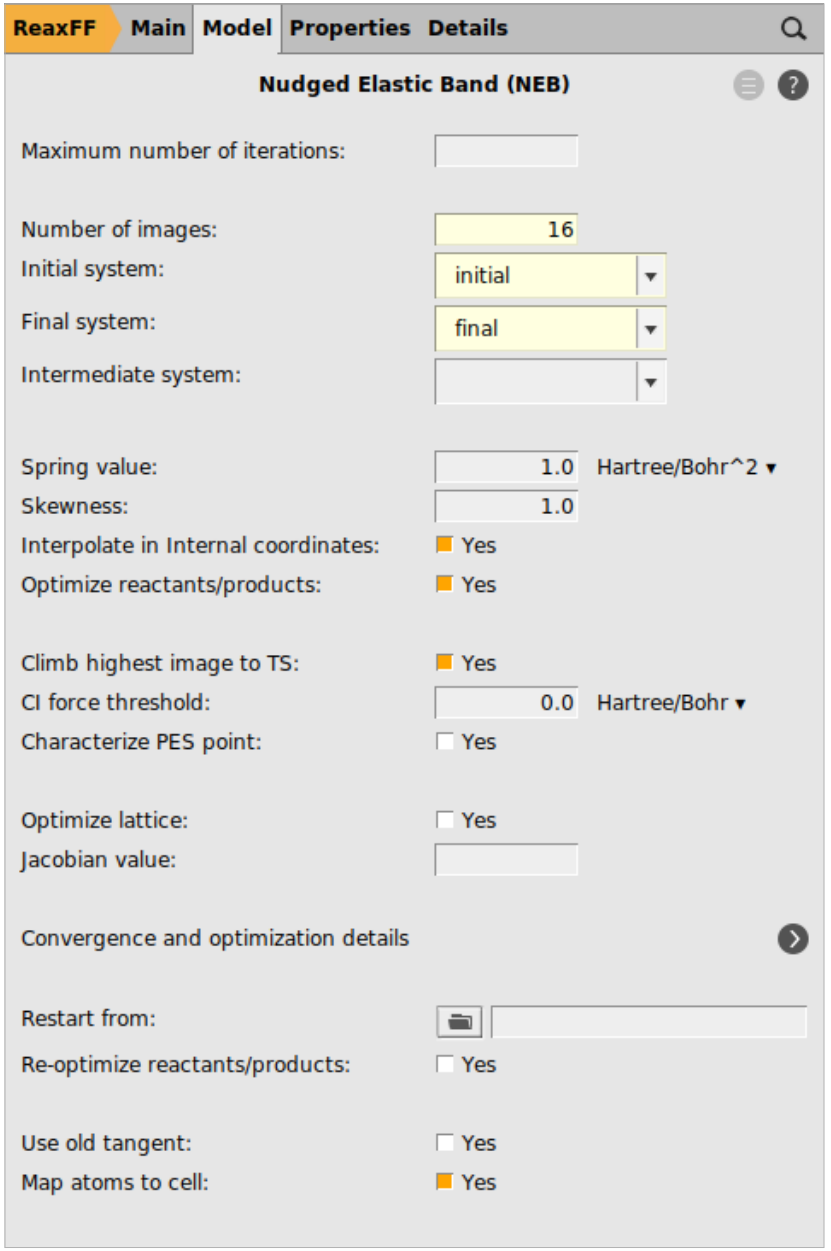
- AMSinput: import ZnOwatersplit_initial.xyz
- **Edit → New Molecule** opens new editor tab
- Switch to **Mol-2** tab and import ZnOwatersplit_final.xyz



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

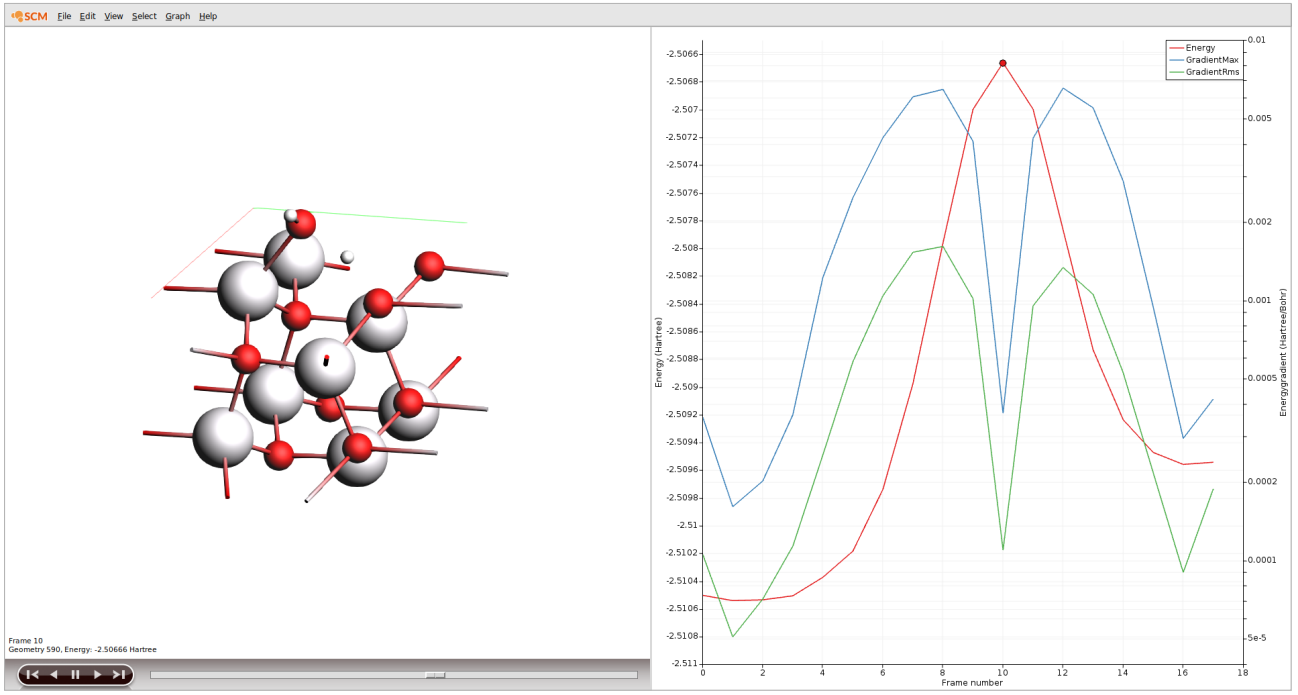
NEB Calculation

- 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