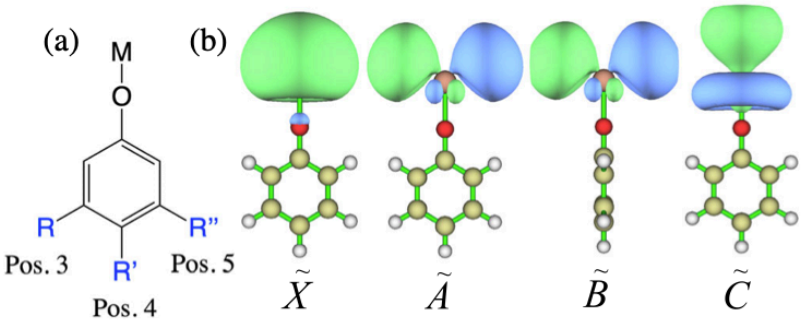
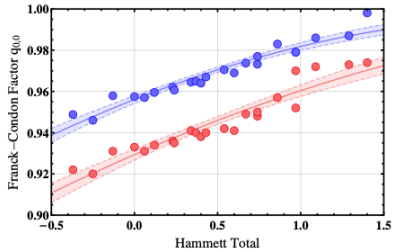
CyberTraining Workshop 2023 project

Taras Khvorost
2023

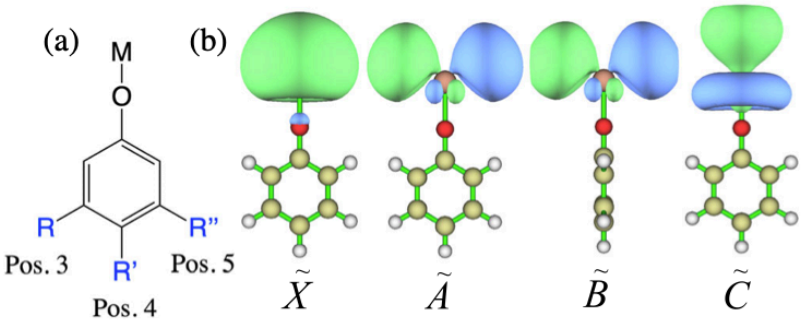
Project idea

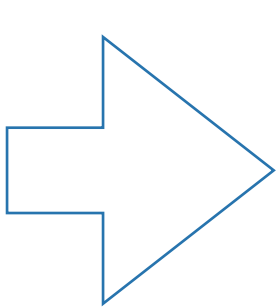


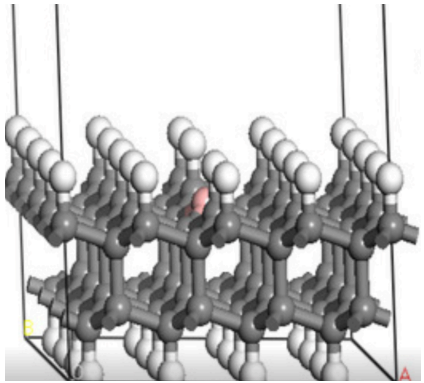


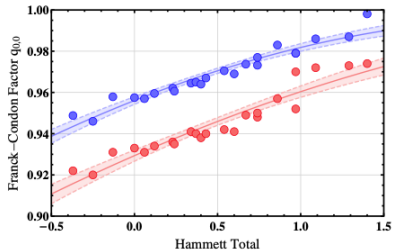
https://doi.org/10.1103/PhysRevLett.126.123002

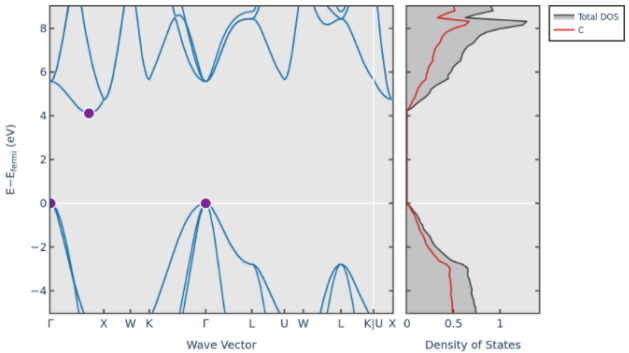
Project idea





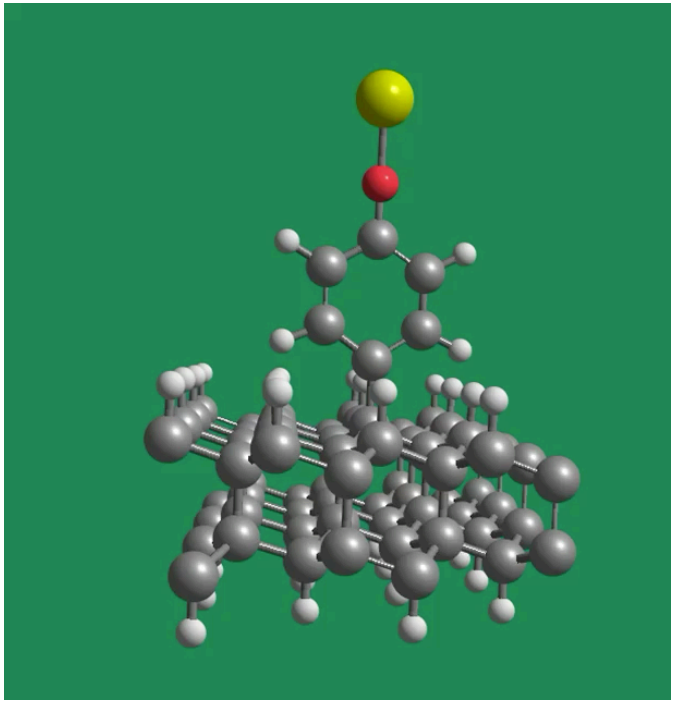






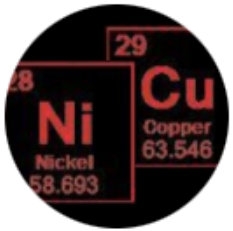
https://doi.org/10.1103/PhysRevLett.126.123002
https://doi.org/10.3390/cryst9080427
CyberWorkshop 2023

Step 1: run md



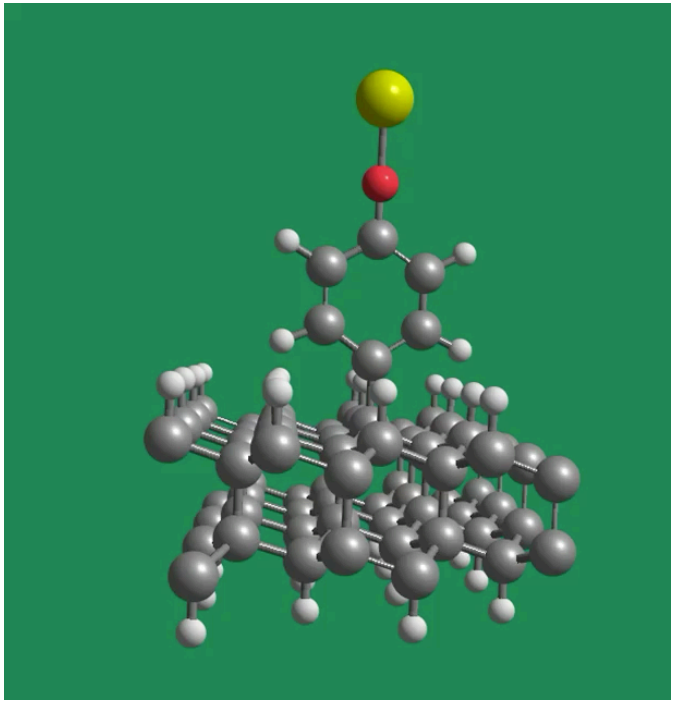
AIMD in CP2K
(Ca: DZVP-MOLOPT-SR-GTH; C,O,H: DZVP-MOLOPT-GTH)
20K, 2000 fs
15 angstrom of vacuum

Unrestricted spin (radical on Ca)!



Nickel and Copper
@nickelandcopper5636 4.32K subscribers 82 videos
More about this channel >

Step 1: run md



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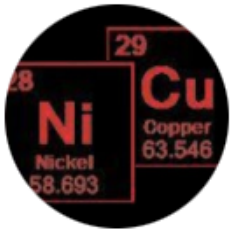

Nickel and Copper
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Step 2: calculate MO overlaps

In [6]:
```
run_slurm = True
submit_template = 'submit_template.slm'
run_python_file = 'run_template.py'
istep = 1200
fstep = 1402
njobs = 30
submission_exe = 'sbatch'
# Removing the previous folders if existed. You can keep them as well
# but Libra will overwrite some of the data if their names are the same
os.system('rm -rf res job* all_logfiles all_pdosfiles')

print('Distributing jobs...')
CP2K_methods.distribute_cp2k_libint_jobs(submit_template, run_python_file, istep, fstep, njo
```

Step 3: calculate NACs?

`params['isUKS']` : A boolean flag for unrestricted spin calculations.

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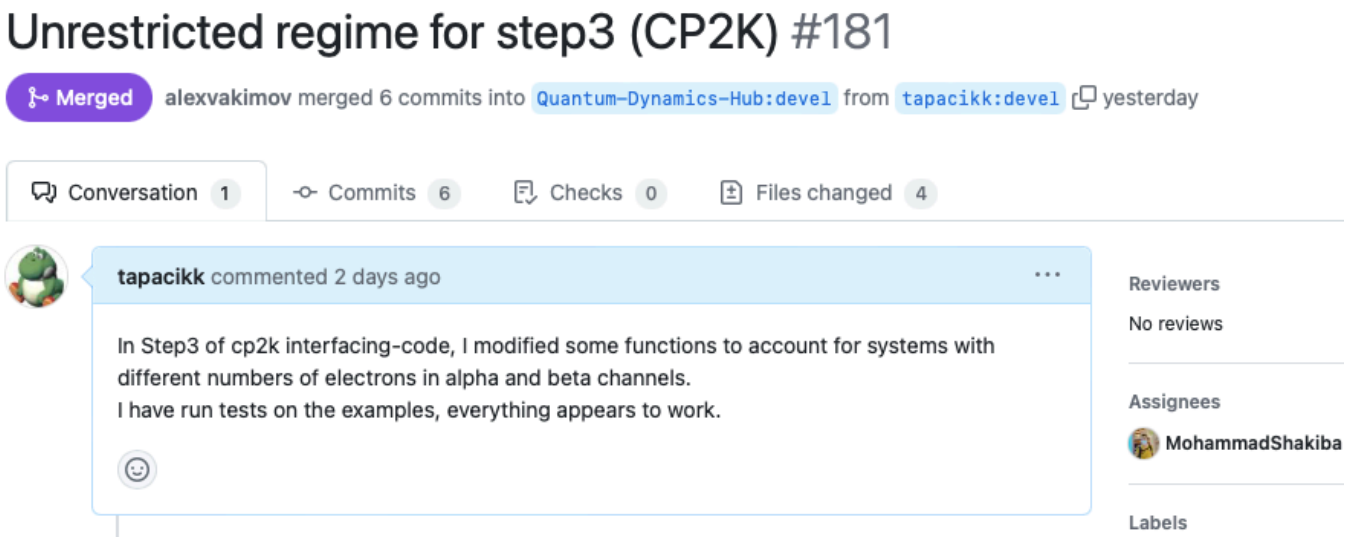


Step 3: calculate NACs?

`params['isUKS']` : A boolean flag for unrestricted spin calculations.

```
params_mb_sd = {
          'lowest_orbital': 166-20, 'highest_orbital': 167+20, 'num_occ_states': 4, 'num_uno
          'isUKS': 1, 'number_of_states': 0, 'tolerance': 0.01, 'verbosity': 0, 'use_multipr
          'is_many_body': 0, 'time_step': 1.0, 'es_software': 'cp2k',
          'path_to_npz_files': '/home/taras/1_example_TiO2/res',
          'logfile_directory': '/home/taras/1_example_TiO2/all_logfiles',
          'path_to_save_sd_Hvibs': os.getcwd()+'/res-mb-sd-DFT',
          'outdir': os.getcwd()+'/res-mb-sd-DFT', 'start_time': 100, 'finish_time': 300, 'so
          'num_occ_alpha': 4,
          'num_occ_beta': 3,
          'num_unocc_alpha': 4,
          'num_unocc_beta': 5
         }

step3.run_step3_sd_nacs_libint(params_mb_sd)
```

Step 3: calculate NACs!

Excited states Active Space

```
0 : [1, -1, 2, -2, 3, -3, 4]
1 : [5, -1, 2, -2, 3, -3, 4]
2 : [6, -1, 2, -2, 3, -3, 4]
3 : [7, -1, 2, -2, 3, -3, 4]
4 : [8, -1, 2, -2, 3, -3, 4]
5 : [1, -1, 5, -2, 3, -3, 4]
6 : [1, -1, 6, -2, 3, -3, 4]
7 : [1, -1, 7, -2, 3, -3, 4]
8 : [1, -1, 8, -2, 3, -3, 4]
9 : [1, -1, 2, -2, 5, -3, 4]
10 : [1, -1, 2, -2, 6, -3, 4]
11 : [1, -1, 2, -2, 7, -3, 4]
12 : [1, -1, 2, -2, 8, -3, 4]
13 : [1, -1, 2, -2, 3, -3, 5]
```

GS

First alpha excited state

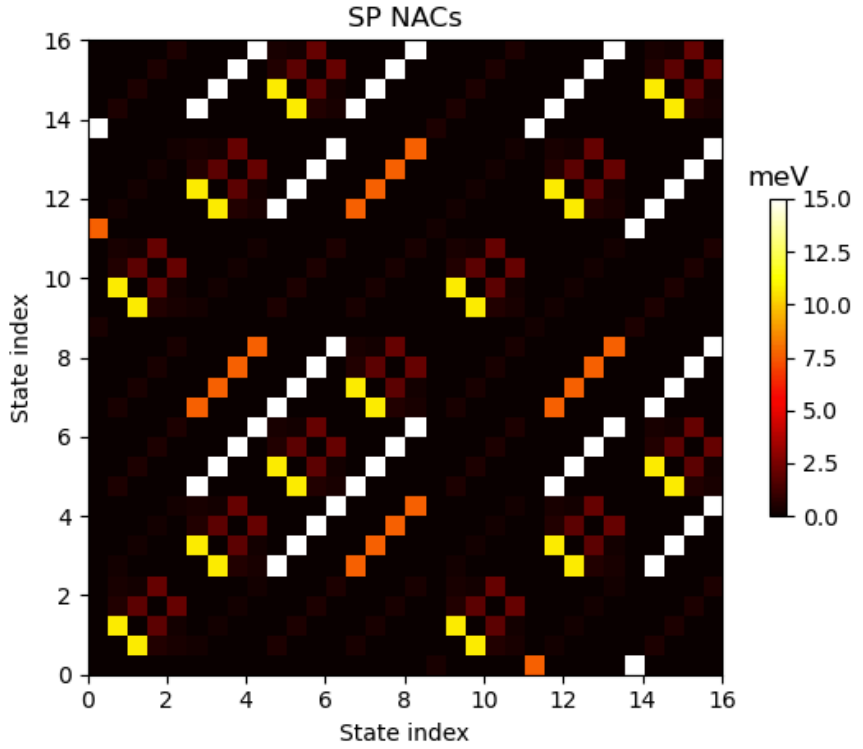
Step 3: calculate NACs!

Excited states Active Space

```
 0 : [1, -1, 2, -2, 3, -3, 4]
 1 : [5, -1, 2, -2, 3, -3, 4]
 2 : [6, -1, 2, -2, 3, -3, 4]
 3 : [7, -1, 2, -2, 3, -3, 4]
 4 : [8, -1, 2, -2, 3, -3, 4]
 5 : [1, -1, 5, -2, 3, -3, 4]
 6 : [1, -1, 6, -2, 3, -3, 4]
 7 : [1, -1, 7, -2, 3, -3, 4]
 8 : [1, -1, 8, -2, 3, -3, 4]
 9 : [1, -1, 2, -2, 5, -3, 4]
 10 : [1, -1, 2, -2, 6, -3, 4]
 11 : [1, -1, 2, -2, 7, -3, 4]
 12 : [1, -1, 2, -2, 8, -3, 4]
 13 : [1, -1, 2, -2, 3, -3, 5]
```

GS

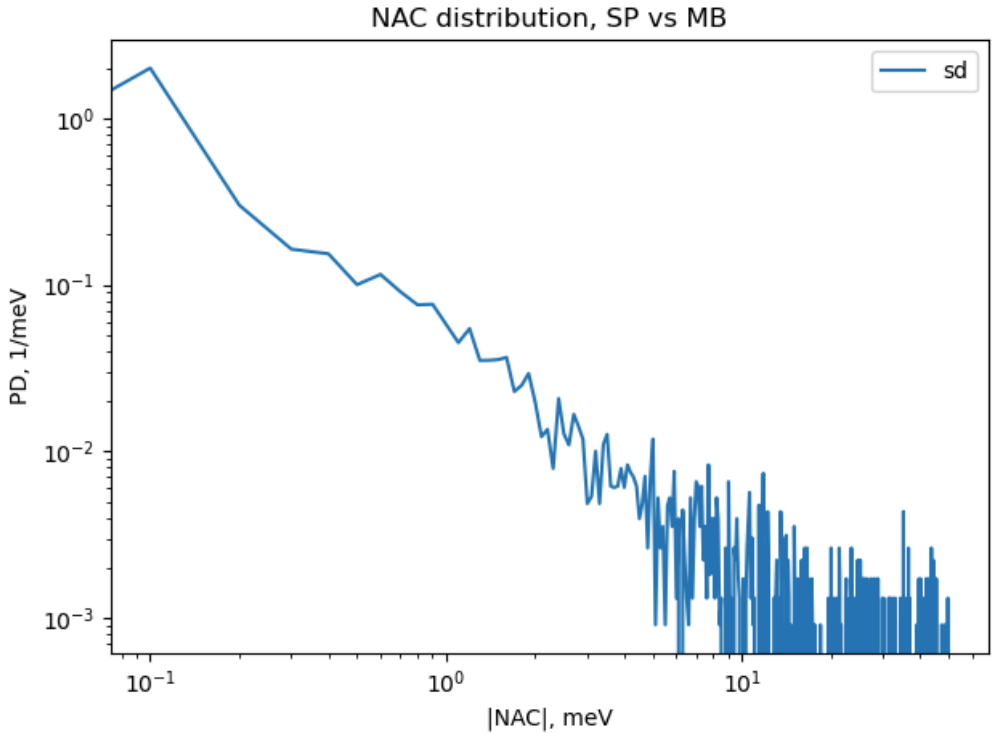
First al

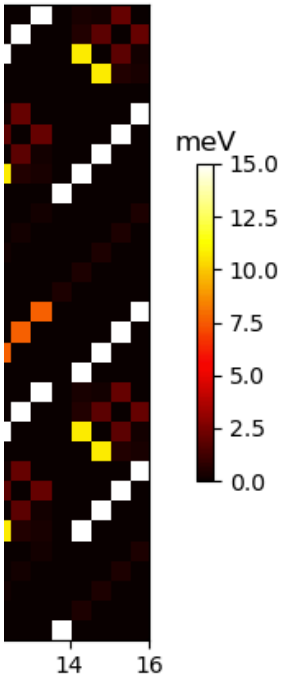


Step 3: calculate NACs!

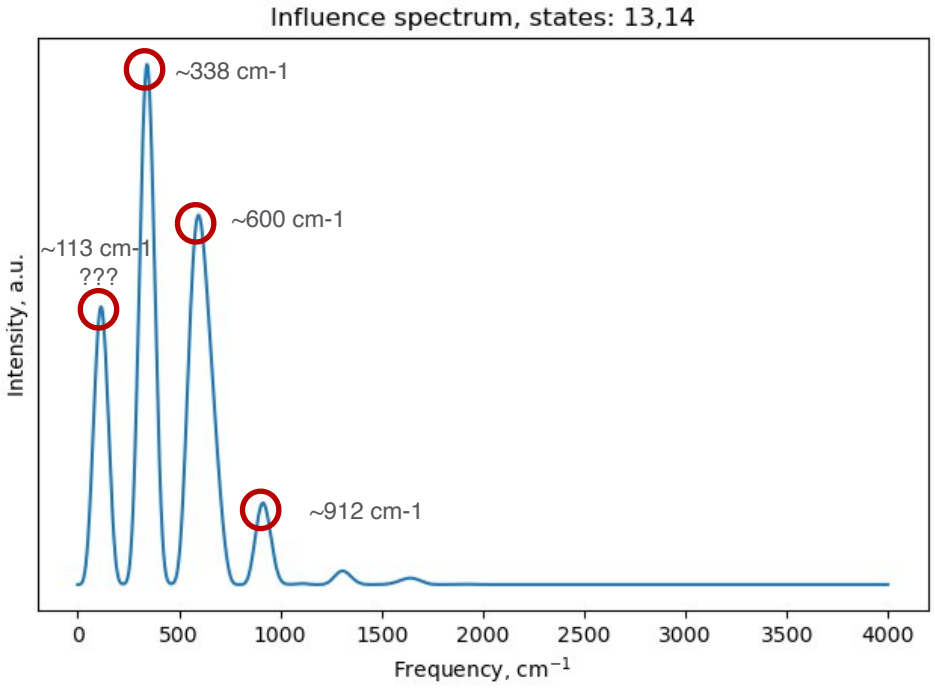
Excited stat

```
0 : [1, -1, 2
1 : [5, -1, 2
2 : [6, -1, 2
3 : [7, -1, 2
4 : [8, -1, 2
5 : [1, -1, 5
6 : [1, -1, 6
7 : [1, -1, 7
8 : [1, -1, 8
9 : [1, -1, 2
10 : [1, -1,
11 : [1, -1,
12 : [1, -1,
13 : [1, -1,
```

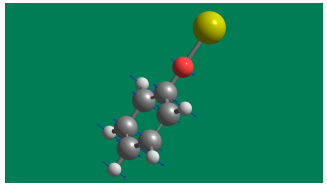




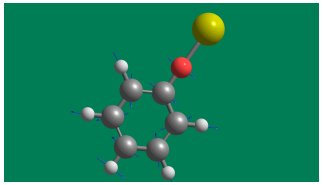
Step 3: influence spectrum



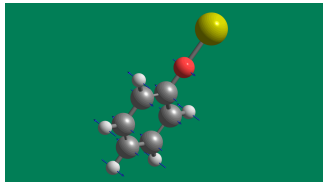
DFT: PBE0/def2-TZVPPD



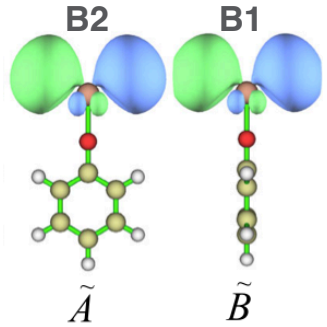
246 cm-1
B1



628 cm-1
B2

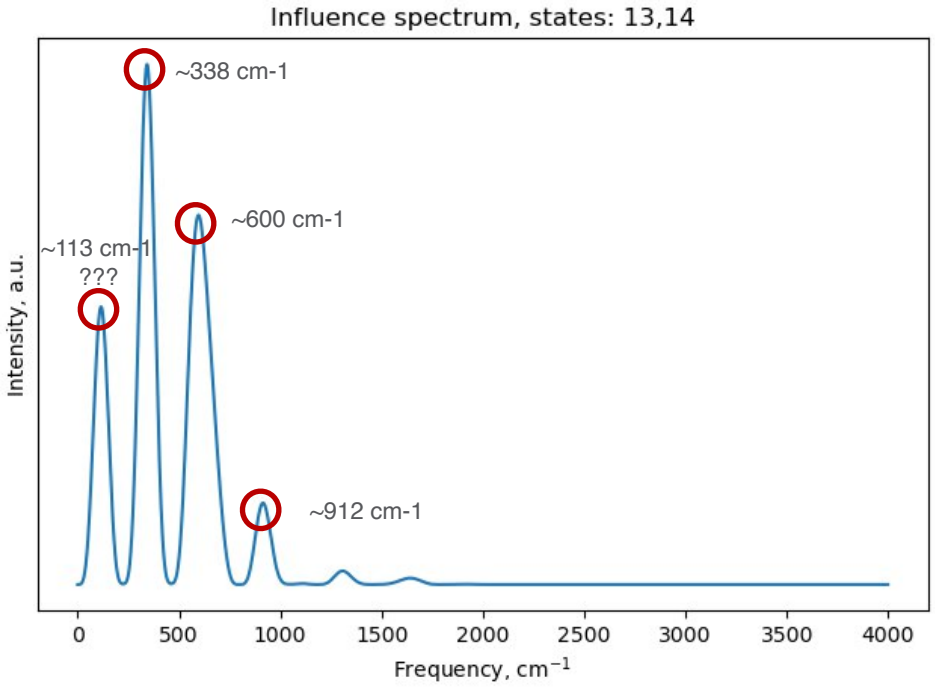


909 cm-1
B1



C_{2v}	E	C_2 (z)	σ_v(xz)	σ_v(yz)	linear f rot
A_1	+1	+1	+1	+1	z
A_2	+1	+1	-1	-1	R_z
B_1	+1	-1	+1	-1	x, R_y
B_2	+1	-1	-1	+1	y, R_x

Step 3: influence spectrum



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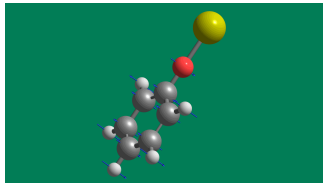

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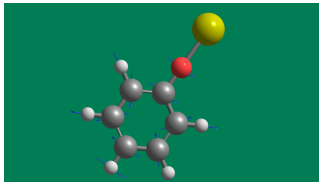
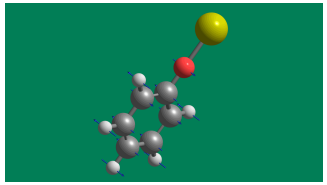


628 cm-1
B2



909 cm-1
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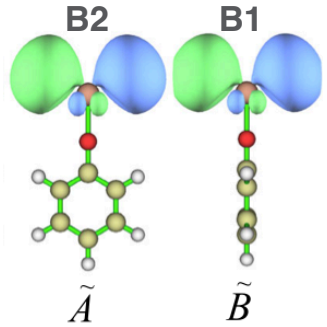
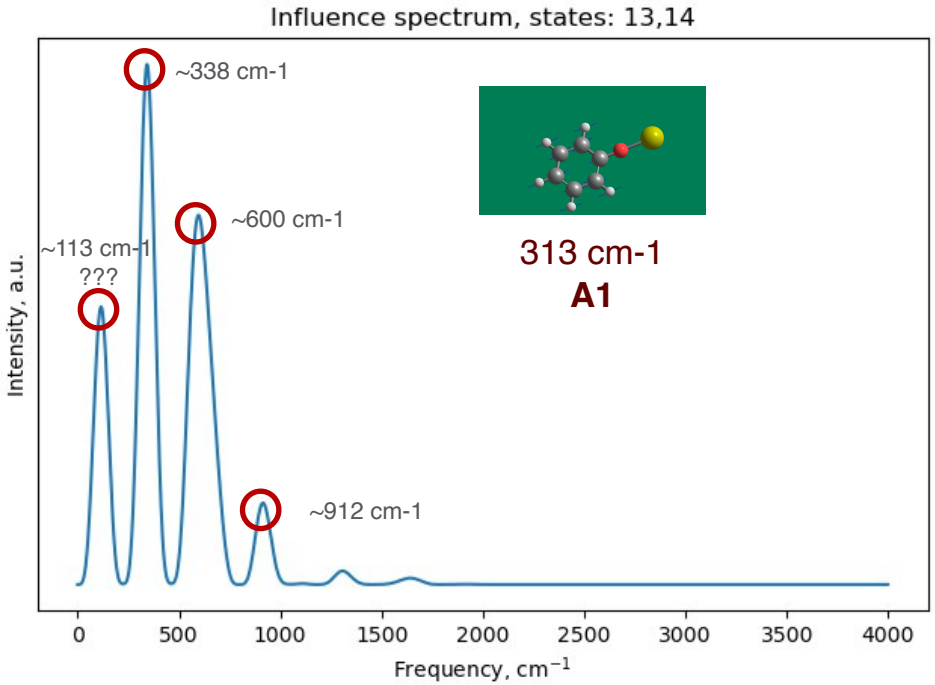


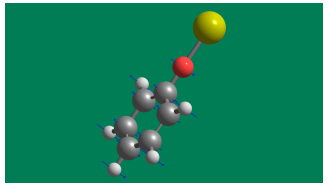
C_{2v}	E	C_2 (z)	σ_v(xz)	σ_v(yz)	linear f rot
A_1	+1	+1	+1	+1	z
A_2	+1	+1	-1	-1	R_z
B_1	+1	-1	+1	-1	x, R_y
B_2	+1	-1	-1	+1	y, R_x

Step 3: influence spectrum



313 cm-1
A1

DFT: PBE0/def2-TZVPPD



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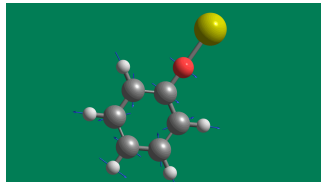
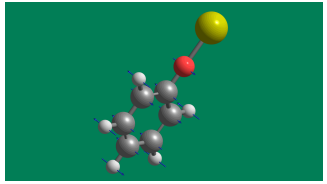
B1



628 cm-1
B2



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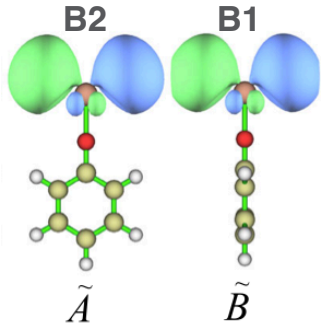

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A_1	+1	+1	+1	+1	z
A_2	+1	+1	-1	-1	R_z
B_1	+1	-1	+1	-1	x, R_y
B_2	+1	-1	-1	+1	y, R_x

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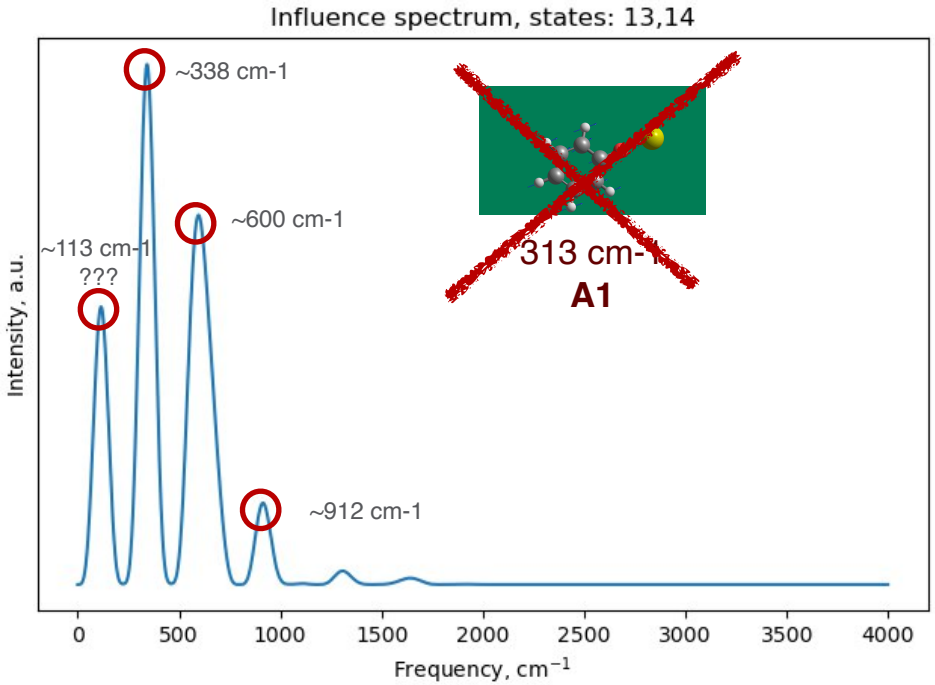

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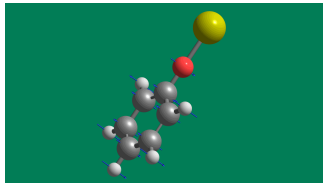
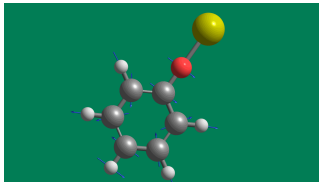
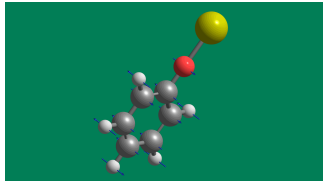


246 cm-1
B1



628 cm-1
B2



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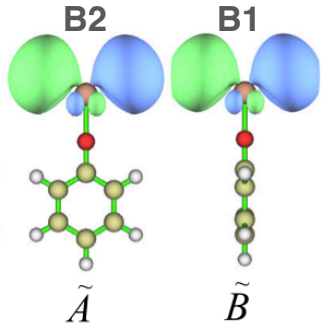

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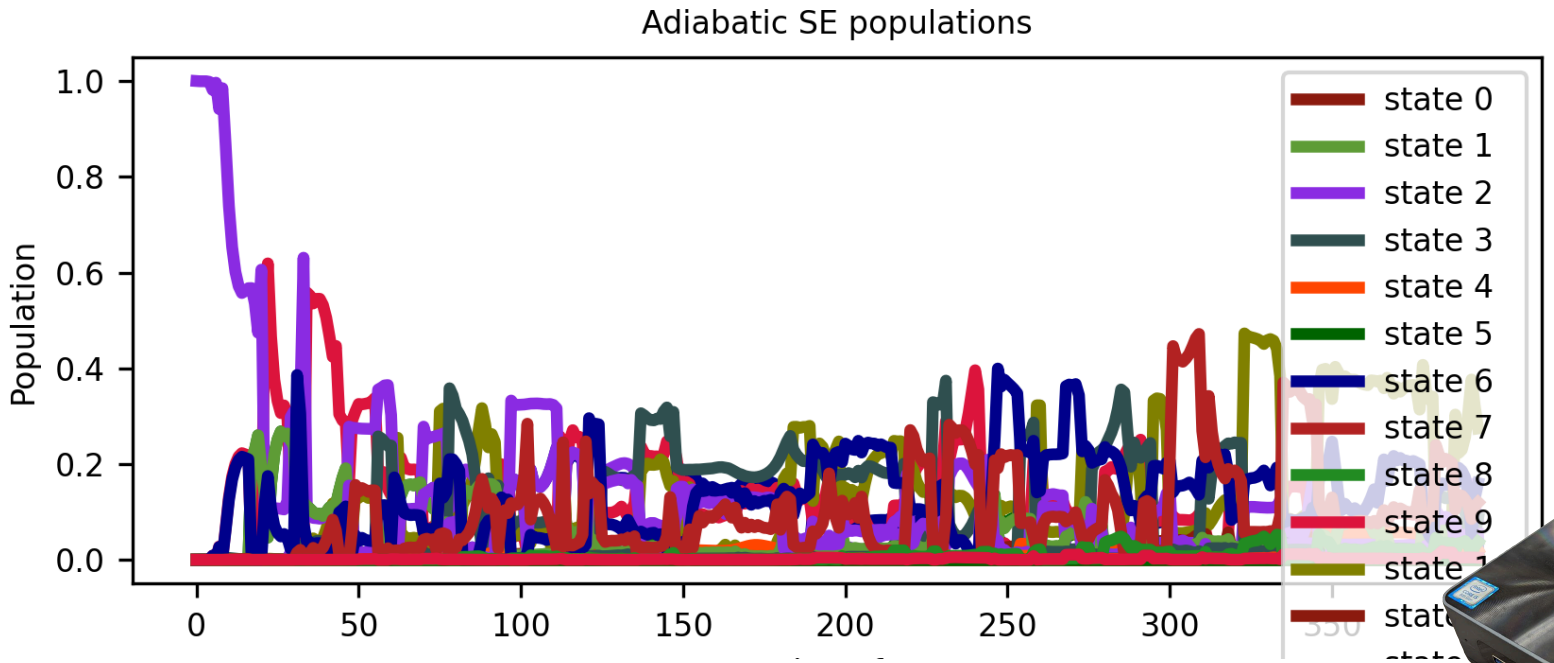
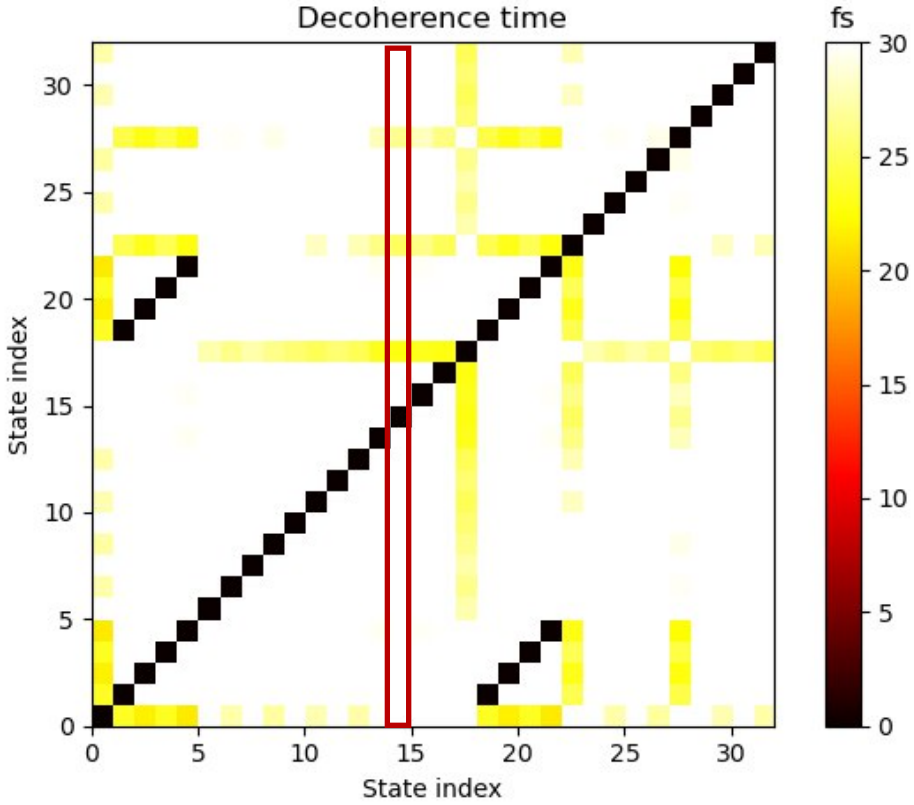
A_1	+1	+1	+1	+1	z
A_2	+1	+1	-1	-1	R_z
B_1	+1	-1	+1	-1	x, R_y
B_2	+1	-1	-1	+1	y, R_x

Step 4


Adiabatic SE populations
Population
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
state 0
state 1
state 2
state 3
state 4
state 5
state 6
state 7
state 8
state 9

Step 4



Thank You