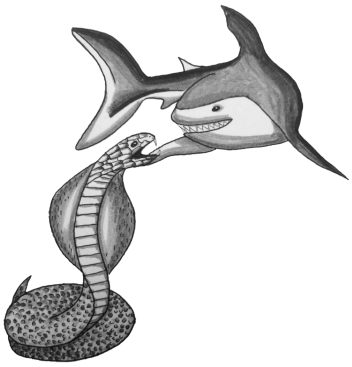
HANDS-ON : SHARC-COBRAMM



We will setup the initial conditions for QM/MM TSH with SHARC/COBRAMM. The system we will solvate with flexible water model is fulvene. Fulvene shows a ultrafast decay (first 40 fs) that can happen through two different conical intersection, giving two different dynamics profile. We will see how sampling differently the initial conditions will change the excited states dynamics.

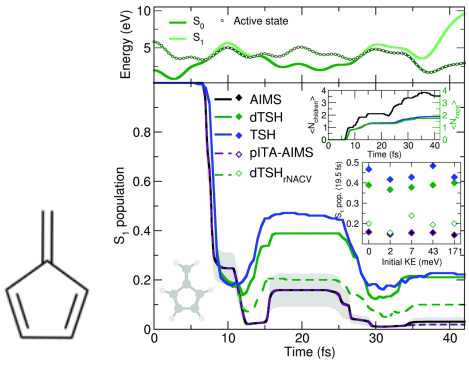


Figure 1 Fulvene molecule used in this hands-on

You can clone from git the necessary material:

git@github.com:compchem-cybertraining/Tutorials_COBRAMM.git

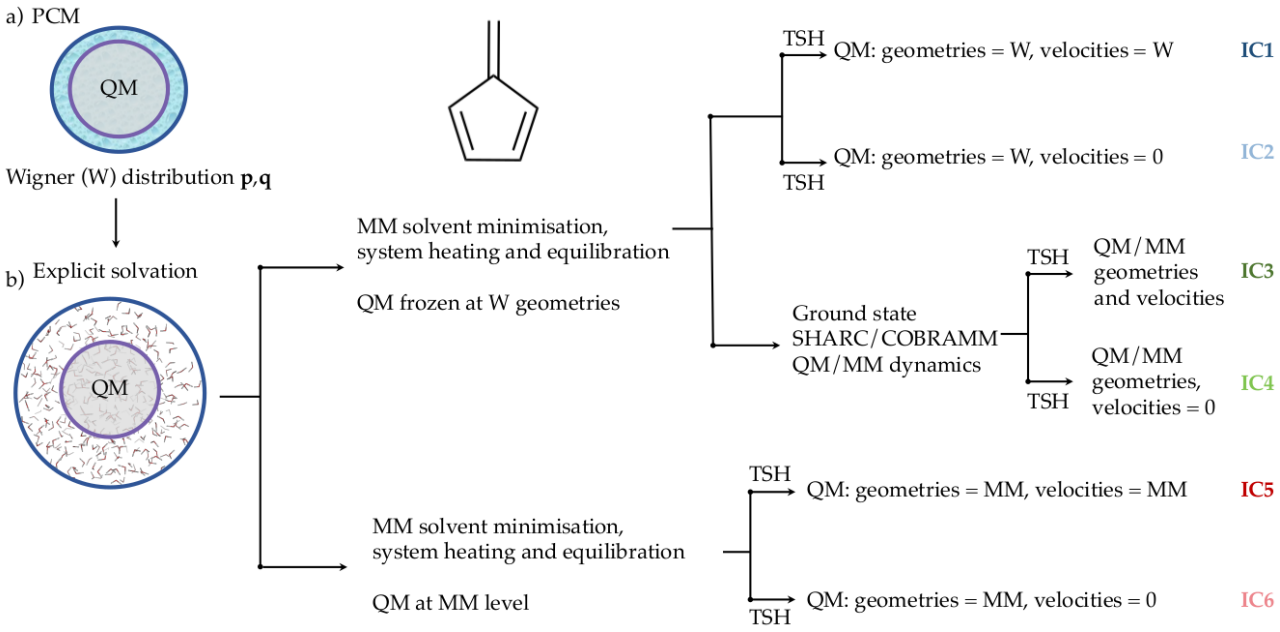


Figure 2 scheme of the different procedure to obtain QM/MM initial conditions

First of all let's setup the system

Write in your bashrc:

```
module load openbabel

AMBERHOME=/projects/academic/cyberwksp21/Software/Conda/Miniconda3/envs/ambertools22/
export PATH=$AMBERHOME/bin:$PATH
export COBRAM_PATH=/projects/academic/cyberwksp21/Software/cobramm
export PATH=$COBRAM_PATH/cobramm:$PATH
export PATH=$COBRAM_PATH/util:$PATH

export SHARC=/projects/academic/cyberwksp21/Software/sharc2.1.1/sharc-master/bin_cobramm
export PATH=$SHARC:$PATH

source /projects/academic/cyberwksp21/Students/smai/Instructors_material/set_openmolcas.sh
```

We can start generating a Wigner distribution for the QM part

```
python2.7 $SHARC/wigner.py -n 10 -t 300 fulvene.freq.molden -x -o initconds_QM
```

and extracting the xyz coordinates

```
sh extract_xyz.sh
```

We will solvate each of the geometries obtained individually

```
cd GEOM_1
```

```
cobramm-solvatedchromo.py -xyz geom.xyz --solvent spcfw -sz 12

sed -i "s/WAT/SPC/g" geom.top

cobramm-equilibration.py -p geom.top -c geom.crd -opt 500 -ht 10 -et 10 –
frozenQM -ctf 4 ###

cobramm-equilibration.py -p geom.top -c geom.crd -opt 500 -ht 10 -et 10 --
frozenQM -ctf 4

cobramm-droplet.py -p geom.top -c finalsnapshot.crd -nm 500 -mr 6
```

copy the COBRAMM input files in the parent folder (only for the first geometry!)

```
cp cobramm_input_files/real.top cobramm_input_files/model-H.top
cobramm_input_files/real_layers.xyz ../
```

once all the geometries are setup, go to the parent folder and run

```
amber_to_initconds.py -t 0.5 -o initconds_MM real.top
GEOM_1/tmpDroplet/input02.crd GEOM_1/tmpDroplet/input02.crd
GEOM_2/tmpDroplet/input02.crd GEOM_3/tmpDroplet/input02.crd
GEOM_4/tmpDroplet/input02.crd GEOM_5/tmpDroplet/input02.crd
GEOM_6/tmpDroplet/input02.crd GEOM_7/tmpDroplet/input02.crd
GEOM_8/tmpDroplet/input02.crd GEOM_9/tmpDroplet/input02.crd
```

call combine_initconds.py and enter the number of QM atoms.

Now we can setup SHARC trajectories as usual, by calling specific setup scripts called

```
setup_cobramm_init.py
```

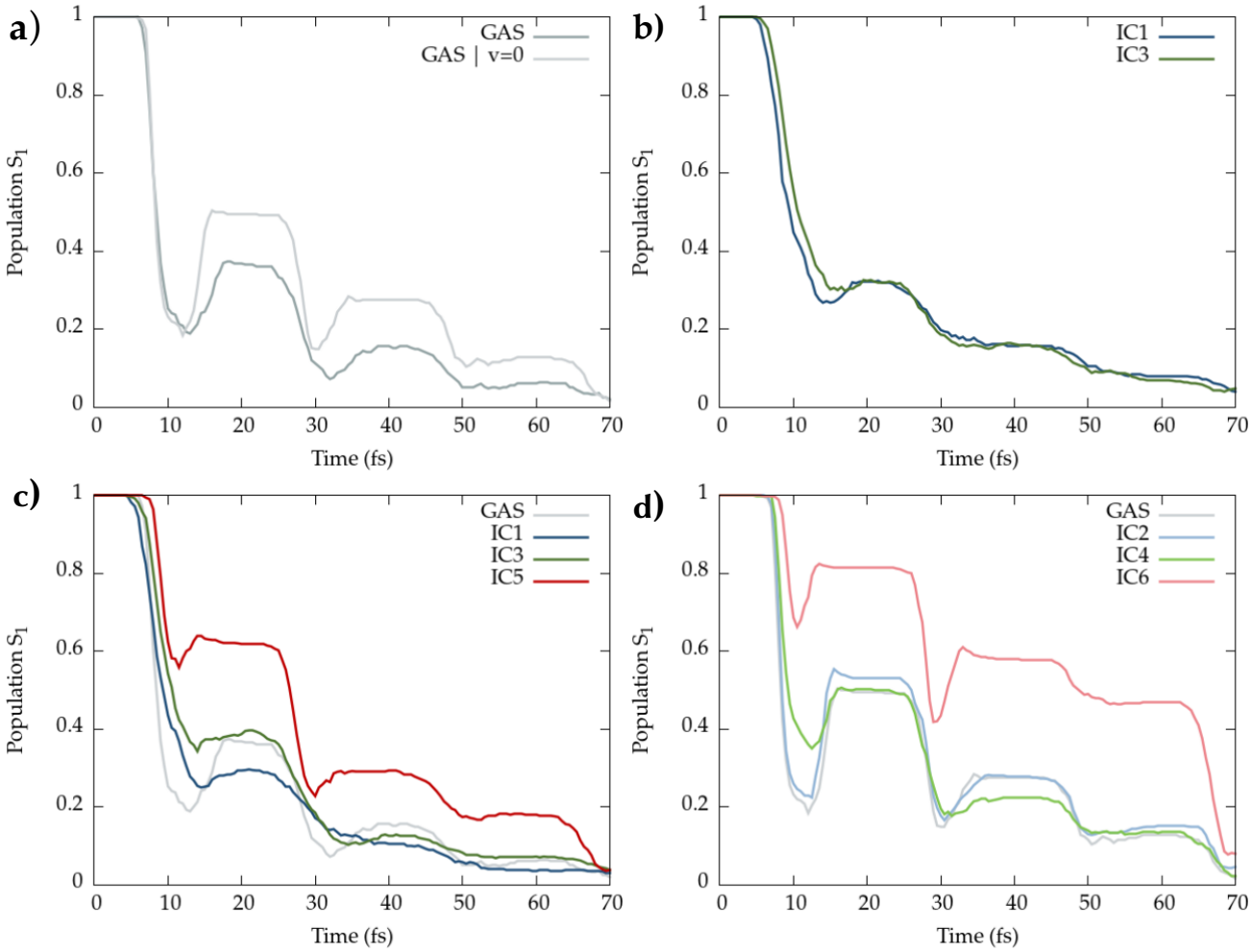
move to ICOND_0000 and run the QM/MM calculation with ./run.sh

```
setup_cobramm_traj.py
```

now you are ready to run your QM/MM TSH trajectories!

DO IT YOURSELF

Generate the set of initial conditions IC3, IC4, IC 5 and IC6. Run 10 trajectories for each of the set and see the differences in the S1 population profile.


a)
GAS
GAS | v=0
Population S_1
Time (fs)
b)
IC1
IC3
Population S_1
Time (fs)
c)
GAS
IC1
IC3
IC5
Population S_1
Time (fs)
d)
GAS
IC2
IC4
IC6
Population S_1
Time (fs)