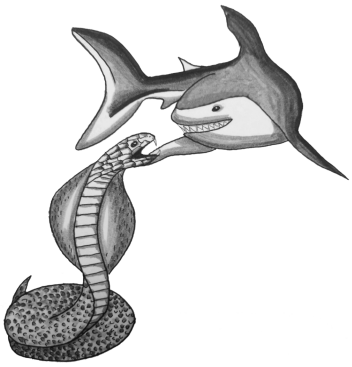
HANDS-ON : SHARC-COBRAMM



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.

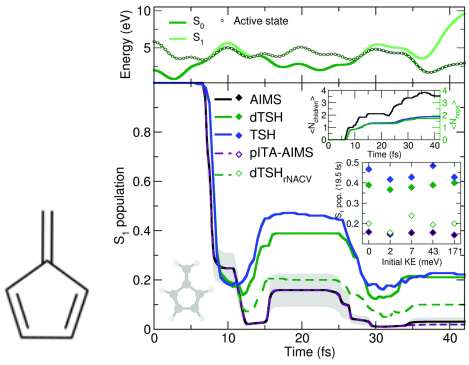


*Figure 1 Fulvene molecule used in this hands-on (**Phys. Chem. Chem. Phys.**, 2020,**22**, 15183-15196)*

You can find the reference work under *Phil. Trans.R. Soc. A*, 2022, 380: 20200381.20200381

You can clone from git the necessary material:

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

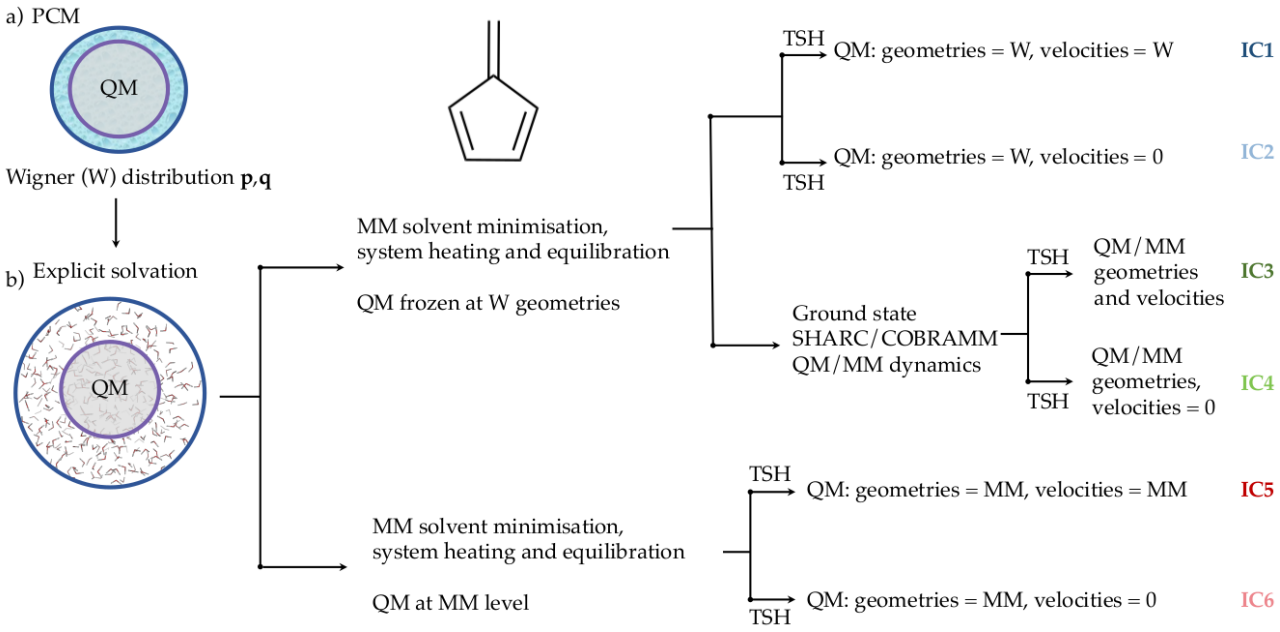


Figure 2 scheme of the different procedure to obtain QM/MM initial conditions

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
```

once the trajectory are setup, you need to manually assign to zero the velocities of the L layers (the last ones in the veloc file) for each trajectory.

```
head -n ($H+M_atoms) veloc > newveloc
for i in {1..($TOTAL-(H+M)_atoms)}; do echo "              0.00000000
0.00000000   0.00000000" >> newveloc ; done
```

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

DO IT YOURSELF

Generate the set of initial conditions IC2, IC3, IC4, IC 5 and IC6. Run 10 trajectories for each of the set and see the differences in the S1 population profile.

In order to run IC3 and IC4, you first need to setup and run SHARC trajectories in the electronic ground state (100fs). Later you can use the script $SHARC/sharctraj_to_initconds.py to generate a new initconds file and setup the trajectories in S_1