CHL Lab

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**QM/MM Protocol**

If you ever need to do a QM/MM calculation, first read the supplemental information section of Xu et al. *J. Phys. Chem. Lett.* **2018**, 2560–2567.

When you are ready, do the following:

1. If you are using fock, the oPM3\_combined in qmmm-files should work. If it does not work or you need to modify the code, re-compile the code.

2. Use rewrite\_residue\_index.sh to renumber the index in your .gro file. Take note of the index of your probe group.

3. Analyze your md trajectory to figure out the distances between each residue / water in system and your probe group, using gmx distance.

4. Use mindisres\*.awk files to process the distance .xvg file, and figure out which residues and how many waters should be included in the QM region.

5. Include the QM residue indexes and number of waters in the input file (qmmm-files/input). Change other options if necessary (see input\_meaning-Layfield.rtf written by Josh Layfield).

6. Put all files in the right place so that qmmm\_sub.sh and qmmm.sh can scan them properly. Run qmmm\_sub.sh to submit qmmm.sh.

7. After you get the output frequency trajectory, analyze it in the same fashion as do column 20 (tot+env) in SolEFP trajectories. The QM/MM output frequencies do not require further modification.

8. Calculate the average frequency as an input to ir-md-ftir.sh; modify and submit ir-md-ftir.sh to calculate lineshapes.