CHL Lab

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**Lineshape Conversion Protocol**

The lineshape conversion script is completely included in the job submission files (ir-md-ftir.sh).

For the thiocyanate probe, 100 fs spacing (dt) in md sampling and ~12 ps delay time in response function (Jct) cut off is sufficient to obtain a converged lineshape. For the trajectory length, the minimum required is ~1 ns, while 5-10 ns is usually sufficient for a converged lineshape.

However, for a different probe, you might need to do some scaling of dt and delay to figure out the optimum value. The rule of thumb is that, you want dt to be as large as possible, so that you are doing solefp calculations on as few frames as possible; however, you do not want dt to be so large that the lineshape does not converge. For delay, in general the long the delay, the better the convergence; however, a delay time that is too long might result in wiggly lineshapes, as the Jct is averaged over fewer data points at longer delay times. In general, figure out a dt first before doing scaling on delay.

The current entry in ir-md-ftir.sh uses a 100 fs spacing for dt, but does scaling (4 ps, 8 ps, 12 ps, 16 ps) on delay.

When you are ready, do the following:

1. Modify ir-md-ftir.sh to reflect the name of your protein, site of mutation, sampling point (spoint) along a trajectory (or ensemble), length of simulation (or your own simulation identifiers). Enter the average frequencies you obtained, in order corresponding to your simulation identifiers, in w.

2. Collect all output \*Jct\*.dat and \*fitr\*.dat and put them in the same directory.

3. Use xmgrace to visualize the scaling. For example, if you are scaling on delay, first visualize the Jct with the longest delay time. Then, overlay multiple ftir files, with the same dt but different delay, by typing xmgrace, followed by multiple filenames. See how the lineshapes are converging as delay time increases.

Refer to the supplemental information section of Xu et al. *J. Phys. Chem. Lett.* **2018**, 2560–2567 for an exampling of scaling.