CHM676 Final Project

1 Objective

The objective of the final project is for you to learn in some detail about an experimental spectroscopic method that interests you. During the project, you should learn about four specific learning objectives

1. The *physical basis* of the technique
2. The *instrumentation* needed to make the measurement experimentally
3. The numerical and theoretical tools needed to *analyze and interpret* the experimental data, and
4. The preparation of *publication-ready figures and text* presenting the data.

It is entirely acceptable – but not required – to model your analysis on a particular paper chosen from the literature. If you do so, **be sure to specify the paper in your write-up!** Do **not**, under any circumstances, copy text verbatim from the literature.

2 Content

The submitted content of the project will consist of

- A Jupyter Notebook that (in some form) generates simulated *raw* "experimental data" and processes it to produce publication-ready figures.
- A write-up of *no more* than five single-spaced pages describing the physical basis, instrumentation, analysis, and interpretation of the simulated data.
- A 40-minute presentation, given in class **between Nov. 30 and Dec. 4**, that summarizes the method and your analysis of it.

Although you are generally free to organize the content in whatever way makes the most sense to you, make sure that your *written submission* (write-up plus code) includes clear answers to the questions listed at the end of this document. (You don't have to phrase them as answers to questions. Just make sure that the answers are included somewhere in the written material.)

Your in-class presentation should summarize your work clearly and concisely. You should be prepared to answer any (reasonable) questions about the method posed by myself or the class.

3 Grading

Credit for the project will be assigned based on

- Your *written materials* (including code) (33%)
- Your *in-class presentation* (33%)
- Your contribution to *in-class discussion* of other presentations (34%).

Each presentation will be followed by a 10-minute question/answer period. It is expected that all members of the class will participate in this discussion. For full credit, each student should ask **at least two** relevant, scientific questions during the course of the presentation series. (Hint: As you listen to each presentation, make a list of questions to ask at the end!)

4 Notes

- Your key objective in submitted materials (including the presentation) should be to **demonstrate your ability to understand, apply, interpret, and present the technique**. Beyond that guideline, the project is intended to be flexible enough to let you pursue whatever spectroscopic methods are most interesting to you.
- Choose the project based on what is interesting to you, **not** based on what is "easy". For grading purposes, expectations for the project will be calibrated against the simplicity of the technique. More detail will be expected in projects that focus on simpler methods; less detail will be expected for more complicated methods.
- Although all four learning objects – physical basis, instrumentation, analysis/interpretation, publication – must be adequately addressed, you may choose to emphasize some learning objectives more strongly than others. For example, a particularly detailed discussion of the physical basis of the technique can compensate for a less-detailed description of the instrumentation.
- If you are currently a member of a research group, you **may not** present on a technique that you are currently using in your research. You **may**, however, present on a technique that you intend to develop in the future but is not yet implemented.

5 Questions to Address in Written Submission

Your written submission (write-up plus code) should *at minimum* address the following questions (grouped by learning objective):

1. **Physical basis:**
   - What kind of molecular or electronic dynamics are probed by the experiment?
   - How does the experiment fit into the (non)linear response framework developed in class? (If it doesn't, explain why not!)
2. **Instrumentation:**
   - What kind of instrumentation is needed to perform the measurement?
   - What is the raw "signal" in your experiment *as measured by the detector(s)*?
3. **Analysis and Interpretation**
   - How is the raw signal processed to produce human-readable images or data?
   - How does the data provide new scientific insight?
4. **Publication:**
   - How has this method been used historically in the literature?
   - What kinds of problems is it being applied to now?