

## CCB 521: Term paper and presentation instructions

### Written report

Each student will prepare a written paper, describing an study involving atomic and molecular structure. You should choose begin by finding a review article that provides background for the subject matter you are interested in. Next, choose one research paper that has a “materials and methods” section (or equivalent) giving details of how the modeling was done. You are encouraged to choose a paper relevant to your area of research that describes a non-trivial application of quantum mechanics. Prepare a careful analysis of the material in the research paper (*not* the review article!) that addresses the following points:

1. Give a brief but clear summary of what was done; it is appropriate to include figures or tables taken from the paper you chose. This should be about 3-4 pages in length. The focus of this analysis should be on the modeling or methods that are used, but you should also describe the context or background involved (*e.g.* experimental results that are being interpreted.) You can use information from the review article as well to provide context here.
2. Describe (in your words this time, and in 1-2 pages) what was learned, and how this analysis was useful to the overall paper.
3. Provide (again, in 1-2 pages) a careful analysis of the strengths and weaknesses of the method as used in this example. Were alternatives available? How much effort went into doing the analysis?
4. Write for an audience of your fellow students, making a real effort provide clear explanations of what was done. The total length of your report should be 6-8 pages, not including citations and figures.

*What you should be doing now:* Think about a topic and papers you want to use; ask your advisor for advice, if appropriate. I want to schedule a (short) one-on-one Zoom meeting with each student between March 20 and March 31 to go over the review article and the paper you have chosen, to answer questions and to provide some direction. Email me a rough draft by **April 24**; we will meet again via Zoom to discuss possible revisions or extensions during that week.

The final paper is due on **May 4** (the first day of finals). Please submit your paper to me via email, as a single pdf file named `lastname.ams.pdf`, substituting in your last name.

### Oral presentation

1. Prepare a 20-25 minute slide presentation on your chosen paper. The presentation should provide background on the scientific context, should describe the methods used, and should explain how modeling helps one to understand its chemical or biological function. The intended audience is your fellow students, not the instructor: work hard to be clear, to explain unfamiliar concepts, and to serve an educational purpose for the class.
2. You may use or adapt figures from the literature, with proper attribution.
3. Presentations will be given in class on **April 26** (Zhu, Kulkarni), and **May 1** (Martin, Dong). Please let me know if there is any reason you cannot attend class on those days. All students are expected to attend each presentation, and to participate in discussion.