24-623/12-623: Case Study Report and Presentation

Objective
The ability to read, understand, and critique papers from the scientific literature is a key skill for any researcher. The purpose of this case study is for you to take the information you have learned in class and critically apply it to published work in the field of molecular simulation. People do amazing things with molecular simulations, but one must carefully inspect the underlying details to have full confidence in reported work.

Task
Pick 3-4 papers related to molecular simulation from peer-reviewed research journals. Prepare a 6-8 page report on these papers and give a 15 minute presentation to the class.

Each student will also prepare a 1-page summary of another student's presentation. You will be told which student you are responsible for.

Evaluation
The case study is worth 25% of your final grade. The written report and oral presentation are each worth 11%, and your one-page summary of another presentation is worth 3%.

Choice of Topic
Ideally, your topic will be something related to your research and/or general interests. The method used in the papers you choose may be MD, another approach (e.g., electronic structure calculations, Monte Carlo methods) or multi-scale modeling involving MD and something else. You must pick papers from at least two different research groups. At least one of the papers must come from outside of your research group. You cannot be the author of any of the papers. Students who happen to choose a similar area for their case studies may have at most one common paper.

Time Line
A summary of your planned work in a pdf file is due at midnight on **November 16** through Blackboard. This document should list the papers to be reviewed and include one paragraph describing the problem you are considering.

All reports are due in a pdf file at midnight on **December 16** through Blackboard. Your report should be between 6 and 8 pages and address the following issues:

- The motivation of the work and details of the simulated system.
- Simulation details. For example, for an MD study, you should describe the interatomic potentials, ensemble, cutoff scheme, thermodynamic conditions (temperature, pressure, etc.), and any other relevant features.
- Special analysis tools used (e.g. Green-Kubo method for thermal conductivity prediction).
- Important results and conclusions.
- Comparison between the methods/techniques/results of the different papers.
- Your opinion of the work and anything else you feel is relevant.

The organization is up to you. Your objective is to report on what has been done and to evaluate the methods used and conclusions reached. I want to see that you have considered the material critically and are not just summarizing it. You will not be penalized for making "wrong" statements, but you should be able to back up whatever you say in a logical manner. You may copy and paste graphics from the papers into your documents, just be sure to properly reference. Email a pdf of the papers being reviewed to McGaughey.

The presentations will take place in class on **November 30 and December 2, 7, and 9**. The full schedule will be available soon. Each student will give a 15 minute talk and have 5 minutes of questions from the audience. You may not be able to cover everything in your report in this time. Try to prepare a presentation that will be accessible by all class members.

Your 1-page summary of another presentation is also due in a pdf file at midnight on **December 16** through Blackboard.