

## Project Proposal

I encourage you to come up with your own ideas and do projects that are part of other research in which you are involved or just areas you find interesting. In general, projects should involve some use of existing codes or writing your own. Just a literature review on a subject is not sufficient. Projects based on other research projects you are doing are encouraged. Projects should represent about 20h of work/person, although more is welcome.

We will work in groups of about 2. I will assign these based on interest expressed in the [Project Information Form F24](#).

### Project proposals should

1. Be about half to a full page and describe what you plan to do.
2. Include a title for your project, your name(s) and a date.
3. Include the codes you plan to use (e.g., LAMMPS), and any languages you plan to use for programming (e.g., Matlab), and any databases you intend to use (e.g., for fitting in machine learning).
4. Include a plan to validate your work by comparison to one or more of an exact theoretical calculation, a previous paper, or an experiment. Other methods of validation might be appropriate in addition or in place of these but please explain them.
5. Be uploaded to canvas.

### Some project ideas

1. Write your own codes
  - 1.1. Write your own MD/MC code to treat a set of atoms in NVE/NVT or other ensembles.
  - 1.2. Write a simple code for a method, e.g., solving a quantum problem, MD, MC, phase field.
  - 1.3. Write a code to treat the Ising or Heisenberg model with MC and calculate magnetization vs. temperature.
2. Use DFT to
  - 2.1. Study electronic properties (e.g., band structure, density of states, magnetism) of a material of interest, e.g., changes in magnetism with strain, surface electronic states, defect states (e.g., donor and acceptor states in Si), magnetic semiconductors.
  - 2.2. Get elastic properties of an alloy vs. composition (e.g.,  $\text{Li}_x\text{Al}_{1-x}$ ).
  - 2.3. Study the stability of high pressure polymorphs and look for pressure induced phase changes, e.g., of Si, SiC, or MgO.
  - 2.4. Study defect energies, e.g., vacancies in graphene.
  - 2.5. Study 2D vs. 3D electronic structure.
  - 2.6. Study phonon properties of a material

- 2.7. Study magnetic phase transition of a material under strain
3. Use LAMMPS
  - 3.1. Explore convergence of MD with time step.
  - 3.2. Explore convergence of MD with systems size, simulations time for melting hysteresis.
  - 3.3. Calculate a melting temperature by direct MD simulations vs. T and simulation of a solid/liquid interface in one cell.
  - 3.4. Calculate temperature dependence of key properties like elastic constants, vacancy energies, and thermal expansion with MD.
  - 3.5. Study effects of nanoscale particles: melting temperature, Gibbs-Thomson energetics, equilibrium shape.
  - 3.6. Assess accuracy of potentials for bulk, surfaces, defects, melting, etc. properties.
  - 3.7. Calculate diffusivity of a liquid using time correlation functions.
  - 3.8. Get free energy (e.g., thermodynamic integration) and see if you can get free energies for a simple case.
  - 3.9. Get activation barriers to atom hopping and predict diffusivities (LAMMPS will allow a more complex calculation).
4. Use Informatics to
  - 4.1. Predict glass forming ability properties.
  - 4.2. Predict band gaps.
  - 4.3. Explore new stable compounds in certain composition space.
  - 4.4. Find correlations in data sets on Citrine database, in Materials Project, etc.
  - 4.5. Identifying Steel Surface Defects With Deep Learning
5. Use some outside code
  - 5.1. Feel free to do a calculation with some other codes or methods than used in the class, e.g., tools for modeling magnetic domains like Vampire (<https://vampire.york.ac.uk/>).

## Final Project Requirements

**Presentation:** 10min. presentation in power point to be given during at the end of the semester (last few classes and even final exam period may be used). Then there will be about 3-5 minutes of questions per presentation. Please practice your talks to make sure they are 10 min. and not over, since we generally have limited time. A rule of thumb is at most one minute per a slide but see what works. The presentation should include

1. A brief introduction to the problem.
2. A description of what you did and problems you encountered.
3. A description of what you learned (can include scientific facts, numerical issues, how certain codes work, etc.).
4. A discussion of what might be done to make further progress on your problem.

You should plan to present from the computer on the podium in the room, not connect your own computer. I will download the talks to make this easy. If you change your title from what I have on the schedule that is totally fine - it is based on the submitted plans and much may have changed since then. Also, please have all members of each group upload the same version of the talk. Please all plan to go up to podium when you present. Ideally all will say something but that is not absolutely necessary.

**Report:** I will ask for a minimum 2 pages of text (single spaced) report about the project. This largely supplements the presentation and summarizes what you did and learned. The report can be longer than 2 pages if you wish. **For group projects each person in the group must submit a separate report which they have written.** Reports for group projects can focus on the whole project or just the portion of the project on which the author of the report focused. In the latter case please include at least a short part in the introduction (can be just a few sentences) describing the overall topic.

Reports should have

1. Clear sections (E.g., these might include Introduction, Methods, Results, Conclusions, or Future Work).
2. Proper referencing.
3. Captions for each figure, table.

Please use any citation style that is convenient for references. That said, I would recommend using one that includes maximal information, e.g, full author lists, titles, and DOIs in the references.

**Grading:** I will grade based on the quality of the presentation, quality of the report, quality of the work accomplished, level of understanding of the problem, and amount learned in doing the work. I realize that all projects are not successful in terms of getting the data for which one had hoped. That is acceptable, but you should make an effort to obtain at least some data and complete some well-defined subproject. If you complete no part of the project, it is hard to give you a strong grade, since I have little sense of what you actually did. If the project is not successful please make an effort to explain what you did and why it did not succeed.

**Deadlines:** All presentations must be uploaded at by the first presentation of the reports no matter when you are presenting. This is fair as people all get the same amount of time. I will deduct credit from anyone who has not uploaded by the deadline to be fair to those who have to present earlier. See the syllabus or online for the specific deadlines.

**A note on late changes to slide decks:** Sometimes people realize after the deadline that they can improve their presentation. This might occur due to seeing some issue while practicing or getting ideas from other talks. Changes might be as simple as a shift in slide order or involve removing and adding significant portions of presentation. I strongly support refining and improving your projects and presentations as this is a great way to make projects better. However, to be fair to those who speak earliest I ask that everyone present what they upload by the deadline. The mechanisms for modification of the presentation after the deadline is to submit to Canvas a revised version with a short comment on the specific changes and the motivation for making them. Then please use the report to describe the change in more detail and tell the

revised story as you would like. This gives everyone a chance to improve their project and presentation through a revised slide deck and the report while still providing consistent and fair deadlines to everyone in the class.

### **Project general suggestions:**

1. Make sure there are clear plans on tasks and everyone has one (can work together). E.g., in a DFT study on ways to get graphene band gaps
  - a. All will work to set up graphene cell.
  - b. Victoria and Emma will study effects on mono- and di-vacancies and B substitution.
  - c. Melanie and Geri will study adatom (O, Cl, F) binding.

### **Project Resources:**

- 1.1. Some useful LAMMPS resources
  - 1.1.1. Visualization and analysis - Ovito, Avagaro (especially for [input files for H2O](#))
  - 1.1.2. Many of you may be considering molecular dynamics or other atomistic simulations and want to know what interatomic potentials are available. Some resources to find ones are below. Please add any other resources you find.
    6. Many potentials are in LAMMPS automatically, can be added from a file, or can be added with parameters taken from a paper.
    7. Here is a database of potentials that may be useful for a quick search to see what's out there: <https://www.ctcms.nist.gov/potentials/>
    8. <https://openkim.org/>
      - 8.1. Note that openkim needs to be compiled with LAMMPS to work. This can be done readily on a Mac with homebrew or on windows with Ubuntu subsystem or on many linux platforms. See this page for info: <https://openkim.org/doc/usage/obtaining-models/>
9. Some useful DFT resources
  - 9.1. QuantumEspresso Tutorials with exercises:  
<https://www.quantum-espresso.org/schools-workshops-tutorials/qesb-2009/>  
  
Videos:  
<https://www.materialscloud.org/learn/sections/Kr5WSY/summer-school-quantum-espresso-santa-barbara-2009>
  - 9.2. Nanohub tools
    - 9.2.1. Nanohub tool for Quantum Espresso:
      - 9.2.1.1. <https://nanohub.org/resources/dftqe> (used in lab).
      - 9.2.1.2. <https://nanohub.org/tools/dftmatprop>
    - 9.2.2. Nanohub tool for AbInit: <https://nanohub.org/tools/abinit>
    - 9.2.3. Try searching “density functional theory” and the filtering on “resources” and “tools”. This gives about 120 tools. Some might suit your needs.
  - 9.3. Guidelines to use codes on Dane Morgan’s linux clusters (Lammp, AbInit DFT code):  
<https://docs.google.com/document/d/19aJPb3GnAgixvjsGtxe9A2uAZEzyRQoF0NMvBFbALMM/edit> (note that you will need to have been given an account so

ask Dane about this). Follow up with Maciej Polak <[mppolak@wisc.edu](mailto:mppolak@wisc.edu)> to get account and more information.

9.4. More information on AbInit DFT code:

9.4.1. Overview: <https://docs.abinit.org/tutorial/>

9.4.2. • [The tutorial 1](#) deals with the H<sub>2</sub> molecule: get the total energy, the electronic energies, the charge density, the bond length, the atomisation energy

9.4.3. • [The tutorial 2](#) deals again with the H<sub>2</sub> molecule: convergence studies, LDA versus GGA

9.4.4. • [The tutorial 3](#) deals with crystalline silicon (an insulator): the definition of a k-point grid, the smearing of the cut-off energy, the computation of a band structure, and again, convergence studies ...

9.4.5. • [The tutorial 4](#) deals with crystalline aluminum (a metal), and its surface: occupation numbers, smearing the Fermi-Dirac distribution, the surface energy, and again, convergence studies ...