

M. Hohle:

Chem 277B: Capstone Project



Timeline

- 1) introduction Oct 28th
- 2) students form groups of up to 5 Nov 4th
- 3) find a project and submit a proposal (HW assignment)
→ reviewed and accepted by us Nov 11th
- 4) checkpoint Nov 21st
- 5) presentations (20min + Q&A)
→ during lecture time/ tutorials week of Dec 6th
- 6) final submission after feedback from presentations Dec 13th
- 7) grading

equivalent to HW assignments

Deliverables:

total: 50% of your grade!

Capstone Project Proposal (5%): 1-2 paragraphs. The proposal will be graded individually on a pass/fail basis (i.e., full credit for passing). If you work in a group, **each of the participants must submit their own proposal**, but please list the other members of your group. Please use the Google Sheet (see **bCourses**) for the group assignment.

Capstone Project Checkpoint (5%): You will need to demonstrate your project status to your GSI in the Workshop section **and** upload your current work to the Capstone Project Checkpoint assignment page. The checkpoint will be graded individually—**each student is responsible for their own submission**.

Capstone Project Presentation (20%): We will schedule demonstrations (individually or with group partners) of the projects to take place during the lecture time of this course. The presentation will be graded as a group; **all members** of your group need to submit the presentation materials (i.e., slides in PDF format and/or Jupyter notebook).

Capstone Project Report (40%): A write-up (see next slide) that would briefly describe your project, algorithm, and any tests you have performed. These write-ups will be graded individually (i.e., **each student needs to submit their own**).

Capstone Project Code Submission (30%): Your primary deliverable is a piece of code and associated data (if any). The project code will be graded as a group, but **each student needs to submit their own**.

Project Report (.pdf):

- Introduction: What is the problem? Why is it important? Brief historical view.
- Methods: algorithms, models
- Implementation: How did you do it exactly.
- Evaluation: Present results in a clear and coherent way.
- Discussion: Interpret results, discuss limits of your model and improvements
- References

Code of Honor:

- Don't copy/paste someone else's (**including AI**) code without citing it!
- It should be **your(!)** work
- Cite, if you use **any** external source
- Not following the code of honor is considered **cheating and will be graded as fail!**

What are possible projects?

last year:

**Tailoring Metal-Organic Frameworks to Uptake
Small Molecule Guests with a Neural Network**

**Predicting Electronic Structure
Properties of Transition Metal
Complexes with Neural Networks**

**Machine learning assisted
crystal recognition**

You can use:

- own data set
- public data (Kaggle, PDB, etc)
- AI support for syntax problems

It must be:

- a **new** problem
- your **own** idea
- worth 50% equivalent
of your grade

What are possible projects?

Evaluation Criteria for Approval:

- **Uniqueness:** Originality of the project concept (reused or open-source code will not be accepted; originality will be verified).
- **Complexity:** Complexity of the project, taking the course timeline into account.
- **Relevance:** Must align with fields such as chemistry, molecular science, or physics, integrating domain-specific insights where possible.

What are possible projects?

Additional Grading Guidelines

- **Plagiarism Monitoring:** All projects will be checked for originality. Direct use of open-source code without modification or attribution will lead to disqualification.
- **Acceptability of Lower Accuracy:** Projects demonstrating a high degree of complexity in dataset selection or model architecture may receive leniency on accuracy requirements, provided the model is well-justified.
- **Research Paper Replication:** Replicating a research paper is allowed if the code used is open-source and modified sufficiently to demonstrate understanding, ensuring that the project is not overly simplistic.

An anonymous survey will be conducted to ensure equitable team contribution. This feedback will help evaluate each member's involvement, ensuring accountability and fairness in grading.



Questions?