**MSE 590400 Homework 1**

Due on **9/18/2025 (Thursday), 23:59**. Upload your homework (pdf, docx, scanned image, etc.) to the drop box of HW01 assignment on the course webpage.

If you use generative AI in your work, you must clearly state it. For example, which AI, briefly comment on what you prompt and what AI tells you.

**1. Semester project pre-proposal**

Goal: In 250–350 words (about half a page), propose a computational materials science problem you will pursue this semester. Whenever possible, choose a topic that meaningfully advances your thesis. If you don't yet have a thesis topic—or if modeling/simulation isn't a natural fit for your current project—select a problem in computational materials that genuinely interests you.

What to include:

(a) Title (1 line): be specific and informative.

(b) Problem (2–3 sentences): What material/system, property, or phenomenon will you study?

(c) Significance (2–3 sentences): Why does it matter scientifically or technologically?

(d) Approach (3–5 sentences): What modeling, simulation method(s), software will you use and why are they appropriate? Examples: DFT, classical/ab-initio MD, Monte Carlo, phase-field, finite-element, cluster expansion, CALPHAD/thermo-kinetic modeling, coarse-grained/continuum.

(e) Planned outcomes (2–3 sentences): What results/quantities/properties do you expect to obtain?

**Note:**

- Don't worry about whether your proposal is fully developed or immediately implementable. The purpose of this assignment is to start a conversation with the instructor. After you submit, the instructor will review your proposal, and you will sign up for a time slot to discuss feasibility, refine the scope, and outline a realistic roadmap for completing the project.
- Use the format for the name of the file you upload: MSE590400_HW1_<project title>_<your name>.<ex>