

CHE384T final project proposal guidelines

Instructions:

Select a research topic for which would reasonable fit within ~4 weeks of work (including a brief literature search, code development, code implementation and debugging, data analysis). The research topic may be related to your own on-going research. You may use code from this course or develop your own code. Use of the off-the-shelf codes may be incorporated but should not be a majority of the project proposed. To make the problem tractable, you may need (and are encouraged) to make a series of assumptions and simplifications, clearly stating each.

Example topics:

- magnetic state transitions with doping
- surface reactions in catalysis
- amorphization of crystalline structure
- constrained molecular dynamics of polymers
- grain growth in polycrystalline structures
- spinodal decomposition of solid-solution materials

Format: 1-2 pages, complete sentences or bullet points acceptable.

Contents:

- Brief intro and background of proposed topic area and research question
- Proposed methodology and approach
- Hypothesis to test
- Proposed plan, e.g., choice of algorithms, code to be constructed, anticipated pitfalls and hurdles