CBE 5440: Final Project Presentation

Each group will present their findings from the final project, covering key aspects of their computational work. The presentation should at least cover the following sections:

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1. Preparation

- **Parameter Selection**: Highlight the selection of the lattice parameter and k-points was studied in HW5. State what you think of the selected parameters.

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2. Surface Modeling and Adsorbates

- **Bulk Cleaved Facets:**
  - Show the **bulk cleaved facets** you generated for your study. Include images and diagrams of the different facets you created (with clear labeling of the Miller indices).
- **Adsorbate Covered Surface Facets:**
  - Discuss the **adsorbates** you ran for the study and their general relevance to the surface chemistry being modeled.
  - Describe the **coverages** of the adsorbates studied.
  - Present images that clearly illustrate the different **adsorbate coverages** on the surfaces.

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3. Pourbaix Diagrams

- **Overview of Pourbaix Diagrams:**
  - Show and explain the **Pourbaix diagrams** you generated for the different facets.
  - Show the general equation used to calculate dG
  - For each facet, clearly identify and explain the **lowest energy adsorbate configurations** you found.
- **Comparison of Facet Diagrams:**
  - Discuss any **similarities/differences** you observed in the Pourbaix diagrams for facets with similar Miller indices.

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4. Symmetric Surfaces

- **Bulk Cleaved Symmetric Surfaces:** Show images of the **bulk cleaved symmetric surfaces**.
- **Surface Energy Equation:** Display the **surface energy equation**

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5. Nanoparticle Generation

- **Nanoparticle**: Each group will be assigned a specific **electrochemical potential**. Show and discuss the **nanoparticles (NPs)** generated at that potential.
- **Comparison to literature:** Do literature search to find any rutile RuO_2 nanoparticles. How does your NP compare to any found in literature?