**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:

**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.

**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.

**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.

**4. Symmetric Surfaces**

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

**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 RuO2 nanoparticles. How does your NP compare to any found in literature?