Istinye University

Faculty of Engineering and Natural Sciences

Department of Chemistry

CHEM409
Capstone Project 1

General Guidelines, Protocols to Be Followed, and Assessment Methods

ISU_MDBF_CHEM_2025_v1

COURSE INFORMATION:

Course Coordinator & Instructor: Assistant Prof. M. Mustafa Cetin (**MMC**)	**Course/Recitation Assistant(s):** - Elif Yılmaz
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Meeting Day, Hour and Room: Fridays (3:00-6:00 pm) in **ANK507**	

ASSESSMENT (Tentative Grading Scale and Course Requirements)*:

Grading Scale	Evaluation Methods	Percent Contribution to Course Grade
AA $\geq$ 90	End of Semester Evaluation (**100 pts total**) (this grade comes from the evaluation table below on the next page)	70%
BA = 80-89	Quizzes (**100 pts total**)	25%
BB = 70-79	Regular Meetings with the Advisor (**100 pts total**)	5%
CB = 60-69		
CC = 50-59		
DC = 45-49		
DD = 35-44		
FF $\leq$ 34	**TOTAL**	100%

*** Borderline grade policy:** I round grades to the nearest 0.50 pts. For example, 89.50 is an AA; 89.49 is a BA.
There are no exceptions to this policy.

CHEM409: TENTATIVE GRADING RUBRIC AND EVALUATIONS

Undergraduate Capstone Project / Graduation Project / Thesis Evaluation Rubric:				
Introduction (15 pts)	**Criterion**	**Description**	**Points**	**Grade**
	Research Problem & Significance (5)	Clearly defines the chemical question, hypothesis, or synthesis target; explains relevance to current chemistry or applications.	0–5	
	Literature Context (5)	Summarizes foundational and recent chemistry literature; highlights knowledge gap being addressed.	0–5	
	Objectives & Scope (5)	States precise aims (e.g., reaction optimization, mechanistic study, material characterization) and expected outcomes.	0–5	
Literature Review (30 pts)	**Criterion**	**Description**	**Points**	**Grade**
	Depth of Research (12)	Integrates authoritative sources (ACS, RSC, Wiley, Elsevier journals, etc.); includes key mechanistic or theoretical background.	0–12	
	Critical Evaluation (18)	Compares methodologies, identifies limitations, and logically motivates chosen approach.	0–18	
Experimental / Computational Methodology (20 pts)	**Criterion**	**Description**	**Points**	**Grade**
	Experimental/ Computational Design (5)	Demonstrates proper planning: reaction schemes, stoichiometry, control experiments, or computational workflow.	0–5	
	Planned Procedural Details (5)	Reports reagents, instruments, conditions, and parameters clearly enough for replication; follows lab safety protocols.	0–5	
	Characterization Techniques (7)	Appropriateness and correct use of spectroscopic/analytical methods (NMR, IR, UV-Vis, GC-MS, XRD, etc.) or computational tools (Gaussian, ORCA, etc.).	0–7	
	Data Management & Error Control (3)	How data (including experimental/computational data) will be managed, recorded, replicated, Proper recording of yields, uncertainties, replicates, and error analysis; ethical data handling.	0–3	
Writing & Formatting (15 pts)	**Criterion**	**Description**	**Points**	**Grade**
	Scientific Writing Quality (5)	Clear, precise, impersonal style; correct terminology and grammar.	0–5	
	Structure & Flow (5)	Logical section order; coherent argumentation from introduction to conclusion.	0–5	
	Formatting & Referencing (5)	Consistent with ACS style; proper citation of equations, figures, and literature.	0–5	
A Proper Two-page Semester Report (20 pts)	**Criterion**	**Description**	**Points**	**Grade**
	Summarizing everything done above	How the work organized, prepared, preparation processes, contribution of each person, and any changes to original proposal for the project	0–20	
		TOTAL	**100**	

Grading Person's Full Name, Signature and Evaluation Date

Full Name :

Signature :

Date :

FURHTER DETAILS REGARDING BOTH CHEM409 and CHEM410

ABSTRACT

DUE DATE: This will be completed after the whole report is complete and evaluated in spring semester within the scope of CHEM410. **Due date and time will be announced in the spring semester.**

DETAILS: 250 words at max - a single image may be used as the graphical abstract

Keywords: keyword 1; keywords 2; … – **5 keywords at max**

This will be completed within the scope of CHEM410.

Essential Components

1. Background (1–2 sentences)

Briefly introduce the topic area and why it matters.

Example: "Metal–organic frameworks (MOFs) have emerged as promising materials for gas storage and catalysis due to their tunable porosity and stability."

2. Objective / Aim

State the main goal or research question of your study.

Example: "This study aims to synthesize and characterize a copper-based MOF for the catalytic degradation of organic dyes."

3. Methods / Approach

Summarize the experimental or computational techniques used — just enough to show scientific rigor.

Example: "The material was prepared by solvothermal synthesis and analyzed using PXRD, FTIR, BET surface area, and UV–Vis spectroscopy."

4. Key Results

Present the most important findings with quantitative details if possible.

Example: "The optimized MOF exhibited a surface area of 1120 $m^2\ g^{-1}$ and achieved 95% dye removal within 30 minutes under visible light."

5. Interpretation / Significance

Explain what the results mean and why they are important.

Example: "The high photocatalytic efficiency demonstrates the potential of Cu-MOF materials in wastewater treatment."

6. Conclusion

End with a one-sentence takeaway or implication for future work.

Example: "This study provides a foundation for designing next-generation MOFs for environmental remediation."

General Tips: Keep it 150–250 words (or as required by your department), use past tense for methods/results, present tense for conclusions. Avoid citations, abbreviations (unless common like NMR, UV–Vis), and detailed data tables. Write it last, after completing the thesis, for best accuracy.

INTRODUCTION

DUE DATE: JAN 9th, 2026 (5:30 pm) – NO EXTENSION TO THIS DEADLINE FOR ANY REASONS.

DETAILS: This will be **100% completed in CHEM409**. Must be clean, precise, strong, and effective, and explain the literature and the State-of-the-Art completely. Students must follow the ACS style citation in the body of the content. Determination of topic, building research question(s), construction of hypothesis, literature search (complete search of literature with relevant information – not a laundry list or not details from Wikipedia and similar sources. Completely scientific search), the State-of-the-Art (what is existing, what is missing, what needs to be done, why your research is important and what gaps it will fill out, etc.).

Key Elements:

1. Background and Context

Introduce the scientific field (e.g., inorganic synthesis, catalysis, analytical chemistry).

Summarize the state of knowledge and why the topic matters (industrial, environmental, biological, etc.).

2. Literature Overview

Present relevant previous studies with concise references.

Identify gaps or limitations in existing research that your work addresses.

3. Research Problem / Hypothesis

Clearly define the research question, problem statement, or hypothesis.

Explain what you aim to discover, verify, or develop.

4. Objectives and Scope

List specific objectives (e.g., "To synthesize and characterize...", "To evaluate catalytic activity...").

Briefly mention the scope — what the thesis covers (and what it does not).

5. Rationale / Significance

Justify why the study is important — link it to real-world applications, sustainability, or technological advances.

Highlight novel aspects or expected contributions to the field.

6. Outline of the Capstone Project / Thesis

End with a short paragraph summarizing the thesis structure, e.g.:

EXPERIMENTAL METHODS, TECHNIQUES AND ETC.

DUE DATE: Please check the dates below.

DETAILS: Given below in each section (**1** and **2**). Please check.

Essential Items (if any of these possible)

1. Experimental Planning, Analytical and Spectroscopic Techniques

This will be 100% completed in CHEM409 and due by **JAN 9th, 2026 (5:30 pm) – NO EXTENSION TO THIS DEADLINE FOR ANY REASONS.**

1.1 Experimental Design and Strategy

- State the **overall approach** to achieving your research objectives (e.g., synthesis route, reaction pathway, or analytical plan).
- Include **reaction schemes**, **flowcharts**, or **process diagrams** showing the stepwise plan.
- Define **variables and controls** (temperature, solvent, catalyst, time, pH, etc.).
- Mention **safety considerations** (hazardous reagents, fume hood use, PPE).

1.2 Reagents and Materials

- List all **chemicals**, **solvents**, and **standards** used with **purity**, **source**, and **catalog numbers** (if available).
- If applicable, describe **sample preparation** (drying, purification, storage).

1.3 Instrumentation and Analytical Techniques

- Summarize the **instruments and methods** used for characterization, with model names and operating conditions:
  - **Spectroscopic methods:** NMR (^1H, ^{13}C, etc.), IR, UV–Vis, fluorescence, Raman
  - **Chromatographic techniques:** GC, HPLC, TLC
  - **Thermal and elemental analysis:** TGA, DSC, CHN analysis
  - **Microscopy or diffraction:** SEM, TEM, XRD, PXRD
  - **Electrochemical methods:** CV, EIS, potentiometry
- State **sample preparation procedures** for each instrument (e.g., KBr pellet for IR, D_2O solvent for NMR).
- Note any **calibration**, **reference standards**, or **blank measurements**.

1.4 Data Analysis and Processing

- Mention software used for **data handling** (e.g., Origin, ChemDraw, Gaussian, MDAnalysis).
- Include **statistical treatment** (averages, standard deviations, regression analysis) if relevant.
- Define how spectra or curves were interpreted and validated.

2. Applied Section (Action Part)

This will be completed after the whole report is complete and evaluated in <u>spring semester</u> within the scope of <u>CHEM410</u>. Due date and time will be announced in the spring semester.

2.1 Step-by-Step Procedures

- Describe **exact experimental operations** concisely but reproducibly:
  - Quantities, concentrations, reaction times, and temperatures
  - Reaction vessels, atmosphere (air, N_2, Ar), stirring rates, etc.
  - Purification steps (filtration, washing, recrystallization, chromatography)
  - Storage and handling of final products or samples

- Avoid copying manual-style instructions; instead use formal scientific language:
  "A mixture of 1.0 mmol $Cu(NO_3)_2{\cdot}3H_2O$ and 2.0 mmol ligand L in 20 mL DMF was heated at 100 °C for 24 h in a Teflon-lined autoclave."

2.2 Characterization of Synthesized or Studied Compounds

- Report **physical appearance**, **yield**, **melting point**, **color**, **solubility**, etc.
- Summarize **key spectral data** (with figure references):
  "IR (KBr, cm^{-1}): 1632 (C=O), 1384 (C–N). ^1H NMR (400 MHz, DMSO-d_6): δ = 7.89 (s, 1H, CH=N)…."
- For materials, include **porosity**, **particle size**, **morphology**, or **thermal stability** data.

2.3 Reaction Monitoring and Optimization (if applicable)

- Describe how progress was tracked (e.g., TLC, UV–Vis, GC).
- Mention how **conditions were optimized** (catalyst loading, solvent screening, temperature effects).
- Present **representative yields or conversion data**.

2.4 Reproducibility and Error Minimization

- Explain how consistency was ensured (triplicate runs, parallel samples, blank corrections).
- Include brief notes on **instrument calibration** or **sample homogeneity**.

General Writing Tips:

Use past tense and passive voice ("was heated," "was analyzed").

Be specific enough for replication but concise enough to maintain flow.

Avoid results or interpretation here — save that for Results and Discussion.

If complex, include an Experimental Flow Diagram summarizing the workflow.

RESULTS AND DISCUSSION

DUE DATE: This will be completed after the whole report is complete and evaluated in spring semester within the scope of CHEM410. **Due date and time will be announced in the spring semester**.

DETAILS:

Essential Items (if any of these possible):

1. Overview of Findings

Brief summary of the main goals and what was achieved.

A sentence connecting results to the research question or hypothesis.

2. Experimental Data Presentation

Key tables and figures: spectra (NMR, IR, UV-Vis, MS), chromatograms, titration curves, calibration plots, yields, etc.

Representative reactions or mechanisms (schemes, equations).

Data should be clearly labeled, numbered, and referenced in the text (e.g., Figure 3 shows…).

3. Data Interpretation

Discuss what the data mean, not just what they show.

Explain trends, anomalies, and comparisons between experimental and theoretical values.

Highlight how the data support or refute your hypothesis.

4. Comparison with Literature

Compare your findings with previously reported results (cite properly).

Identify any novelty or deviation from known studies.

Mention possible sources of discrepancy (instrumental error, reaction conditions, sample purity, etc.).

5. Mechanistic or Structural Insights

Provide reasoning behind observed chemical behavior (reaction pathways, kinetics, stability, electronic effects, etc.).

Use spectroscopic evidence to justify structural assignments.

6. Quantitative and Statistical Analysis

Include calculations, error analysis, or replicates (where relevant).

Report significant figures and uncertainties correctly.

If modeling or simulations were done, summarize key parameters and outputs.

7. Correlation between Sections

Link the results logically to your objectives and experimental design.

End each subsection with a mini-conclusion before moving to the next part.

8. Discussion of Limitations

Identify limitations or uncertainties in your work.

Suggest what could be improved or optimized in future studies.

9. Concluding Remarks

Conclude the section by summarizing the main findings and their significance. Transition smoothly to the Conclusion chapter.

CONLUSIONS:

DUE DATE: This will be completed after the whole report is complete and evaluated in spring semester within the scope of CHEM410. **Due date and time will be announced in the spring semester**.

DETAILS:

1. Summary of Key Findings

Restate the main objectives in one sentence.

Example: “This study aimed to synthesize and characterize a new Cu(II)-based coordination complex for catalytic oxidation reactions.”

Summarize your most important results (quantitative if possible).

Example: “The complex exhibited 90% conversion under mild conditions and showed thermal stability up to 300 °C.”

2. Interpretation and Significance

Explain what your results mean in the context of the broader field.

Example: “The enhanced catalytic performance is attributed to the synergistic effect of the Cu(II) center and the nitrogen-donor ligand.”

Mention how your findings fill a gap, support a hypothesis, or advance understanding of the system.

3. Limitations

Briefly identify experimental constraints or uncertainties (e.g., limited sample size, measurement error, lack of in situ data).

Example: “The catalytic recyclability was tested for only three cycles; longer-term studies are needed.”

4. Future Work

Suggest specific directions for future research.

Example: “Further studies could explore ligand modification to improve selectivity or test the catalyst under continuous-flow conditions.”

If relevant, mention applications (industrial, biomedical, environmental).

5. Final Remark

End with one strong, positive closing statement that emphasizes the overall value of your work.

Example: “Overall, this research contributes to the development of efficient, sustainable metal–ligand systems for green catalytic applications.”

REFERENCES:

DUE DATE: This section is **SPECIAL because both fall and spring semester work will have this section**. Thus, for the **CHEM409**, the due date is JAN 9th, 2026 (5:30 pm) – NO EXTENSION TO THIS DEADLINE FOR ANY REASONS. For **CHEM410**, the due date will be in spring semester (**due date and time will be announced in the spring semester**).

DETAILS:

ACS Style. For further details please visit:

https://pubs.acs.org/doi/full/10.1021/acsguide.40303

"It is mandatory to format citations in ACS style. For detailed rules and examples, please consult the ACS Guide to Scholarly Communication — ACS Style Quick Guide and the ACS Reference Guidelines."

APPENDICES

Purpose: The appendices provide supporting information that is too detailed for the main text but necessary for verification, replication, or deeper understanding of your research. Each appendix should be labeled clearly (Appendix A, Appendix B, etc.) and referenced in the main text (e.g., "Full spectra are provided in Appendix A").

1. Supplementary Experimental Data
Full spectral data
NMR (^1H, ^{13}C, etc.) with chemical shifts, multiplicities, and coupling constants
FTIR, UV–Vis, fluorescence, or MS spectra (include figure captions)
Powder XRD patterns, DSC/TGA curves, chromatograms
Raw data tables not included in the main Results section (e.g., full kinetic data, calibration curves).
Computational or simulation parameters (Gaussian input files, MD simulation details, etc.).

2. Detailed Experimental Procedures
Step-by-step synthesis or preparation protocols (quantities, conditions, reaction yields).
Instrumental parameters (e.g., detector wavelength, scan range, integration times).
Safety or waste disposal notes if not fully covered in the main text.

3. Additional Figures, Tables, and Calculations
Extended figures (SEM/TEM images, spectra overlays, mechanism schemes).
Example calculations (molar yield, rate constants, Beer–Lambert plots, stoichiometric conversions).
Error analysis or statistical treatment supporting the reported data.

4. Characterization Certificates or Supplementary Documents
Instrument output reports (e.g., elemental analysis, ICP–MS reports).
Material or compound certificates (purity, batch info, safety data).
Software-generated outputs (spectral fits, simulation trajectories).

5. Supporting Literature and Additional Information
Extended literature tables (comparison of your results with literature values).
Lists of abbreviations, symbols, or chemical structures not included in the main text.
Ethical statements, consent forms, or institutional approvals, if applicable.