Thesis Proposal, Agreement, and Timeline Template

The Thesis Proposal, Agreement, & Timeline, signed and approved by your mentor, should be submitted to the HC via webform. This template offers a guide of what should be included.

Title

Using Grand canonical Monte-Carlo Simulations to Locate Gas Adsorption Sites in Non-Crystalline Nano-Porous Materials

Your Name: Arthur York (SID 932-727-281)

Introduction

Metal-Organic Frameworks (MOFs) are highly tunable materials with high internal surface areas, making them perfect for gas storage applications. There are thousands of known MOFs so finding the ideal candidate for a specific gas through experimentation is unrealistic. Therefore, a way to computationally screen potential MOFs for affinity to different gasses allows researchers to focus on only the most promising materials.

There are many other types of nano-porous materials that are promising for increasing gas storage potentials, such as porous coordination cages. However, these materials are non-crystalline meaning it is difficult to use x-ray diffraction techniques to determine gas adsorption sites. The simulation is verified by comparing experimental and simulated adsorption isotherms. After validation, the location of adsorbates inside the structure is stored to create cloud plots depicting likely adsorption sites.

Thesis Statement /Hypothesis / Goal Statement

The goal of this project is to develop a method for calculating gas adsorption in different materials, and save the location of adsorbate molecules throughout the simulation to find potential adsorption sites.

Approach/Methodology

This project will use the Julia language and build off of the PorousMaterials.jl package to implement a Grand-canonical Monte Carlo simulation. The data from simulated adsorption will be compared to experimental data to ensure the simulation is working correctly. Once the model is working, a range of MOFs will be simulated for methane adsorption. The results from these will be compared to find which MOFs would be most promising for experimental testing.

There are no human subjects involved at any point in this project.

Expected Results/Anticipated Outcome and Significance

This project will yield a simulation that can be used for simulating gas adsorption in MOFs and similar nano-porous materials. After the simulation model has been compared with experimental results, it can be used to capture adsorbate locations and find adsorption sites. This simulation can provide information about the structure and adsorbates when x-ray diffraction and other experimental methods are unreliable.

SIGNATURE LINE

Mentor: _____ Feb. 6, 2020

Cory Simon, (CBEE) Date

By signing, the mentor gives his/her assurance that they have read the proposal, sees it as a legitimate HC research project, and is willing to serve as your thesis advisor for the proposed project. If this project requires IRB approval, the mentor confirms eligibility as a Principal Investigator according to IRB criteria.

Honors College Thesis Expectations Agreement

Student Responsibilities

- Work 3 hours each week per research credit in CHE401 course.
  Students typically work 3-5 hours each week per graded research credit in the discipline of their mentor.
  (i.e. 2 credits of BB 403 is equivalent to 6-10 hours per week)
- Maintain a notebook/journal/lab record to verify accomplishments, protocols, problems, questions, dates and number of hours worked and results.
- Mid-way through the research, student will select committee members (the committee will include the mentor, and two others) to review the thesis. Selection of committee members is in consultation with and approved by the thesis mentor.
- Submit a final draft copy of the thesis to their thesis committee no later than ten business days prior to their scheduled thesis defense date
- Present their thesis in front of their thesis committee, discuss and defend their thesis by answering questions about their research and related topics such as theoretical background, rationale, results, experimental design and overall significance
- Revise, edit, and complete the final thesis and submit to OSU Scholar Archive no later than Friday of week 10 of their graduation term.
- Gather signatures for thesis submission form and submit to the Honors College no later than Friday of week 10 of their graduation term.

Student: Arthur York 6 February 2020

Arthur York — Date

By signing, the student gives their assurance that they agree to the 'Student Responsibilities' outlined for the proposed project.

Mentor Responsibilities

- Provide guidance on the development and direction of the research project. The project, including background reading and real-time research, should take about 18-30 total hours (6 credits at 3-5 hours per credit).
- Explain and demonstrate how records should to be kept, including notebooks or data organization and storage.
- Identify the publishing or style guide to be used for the thesis: IEEE
  o Typical examples are APA, Harvard, IEEE, MLA, etc.
- Recommend a secondary person for the student to utilize in case of questions:
  Árni Sturluson
  Assist in preparing and reviewing:
  - o project timeline
  - o project reference materials
  - o drafts of the written thesis
- Assist in selecting and approving fellow committee members.
- Provide grades for research credits in terms student enrolls.
- Provide guidance as the student designs the poster and prepares for the thesis defense.
- Chair the student's thesis defense.

Mentor: Feb. 6, 2020

Cory Simon, (CBEE) — Date

By signing, the mentor gives their assurance that they agree to the 'Mentor Responsibilities' outlined for the proposed project.

Honors College Thesis Proposed Timeline

General Guidelines: In Stage 4, 1st term - Read & Research / 2nd term -Analyze Results & Write / 3rd term – Edit, Defend & Submit

Suggested Submit Date:		Submit to:
31 Oct. 2020	**Read and summarize past literature on topic**	Arthur
6 Jan. 2020	**Gather questions / research / data / themes**	Arthur
	Finish collecting data by start of winter term	
31 Jan. 2020	**Analyze thesis questions / data / research / themes**	Arthur
	Week 4 winter term	
21 Feb. 2020	**Select committee members**	Dr. Simon
20 Mar. 2020	**Write and format thesis (Rough Draft)**	Dr. Simon
	Finish rough draft by end of finals winter term (7 weeks from end of analysis)	
24 Apr. 2020	**Revise thesis draft #1, #2, #3**	Dr. Simon
	4 school weeks to revise + spring break	
27 Apr. 2020	**Finalized draft to the thesis committee**	Dr. Simon
	10-15 business days for committee to review	
1 May 2020	**Schedule the thesis defense**	Arthur
	Schedule 2 weeks in advance	
6 May 2020	**Design and print the thesis poster**	Arthur
	Turn in for printing slightly before finalizing presentation	
8 May 2020	**Create a presentation on your project**	Arthur
	1 week to practice presentation after finalizing it	
15 May 2020	**Defend the thesis project**	Arthur
28 May 2020	**Make revisions to the thesis and format it**	Dr. Simon
	2 weeks for final revisions after defense	
29 May 2020	**Upload thesis to the OSU Scholars Archive**	Arthur
29 May 2020	**Gather approval signatures**	Arthur
5 June 2020	**Submit the thesis**	HC Office