Medford Group Recruiting Assignment

Deliverable: Please write a one-page mini-proposal based on the project you are most interested in. You should answer the question: If you were given the time and resources, what problem would you want to solve within the scope of the project? What would the necessary steps to solve this problem be? You may use figures if you like, but the entire document should not exceed a page (11pt font, standard margins). You may discuss this with graduate students in the group, but please **do not ask them (or anyone else) to review the written document prior to submission**. Note that you are not technically required to complete this assignment to join the group, but it will certainly help if student selection is competitive. This may also be a good starting point for applying for fellowships such as the NSF GRFP, so hopefully the effort is productive.

Suggested sections and lengths:

- Goal (~1-3 sentences): Most research is either "hypothesis driven" or "objective driven". The goal of hypothesis-driven research is evidence for or against a *falsifiable* hypothesis, while the outcome of objective driven research is a specific deliverable (e.g. a software tool). Think about which type of goal you would like to pursue and concisely describe the specific hypothesis or objective you would seek to achieve.
- Strategy (~2-3 paragraphs): Think about the specific intermediate challenges that will need to be overcome to achieve your goal, as well as the tools you might apply to solve them. Given that these topics are very new to you, I don't expect a lot of technical details. I'm looking to see how you would break a problem down into manageable tasks, but I'm not really concerned about whether the tasks are achievable.
- Impact (~1 paragraph): Briefly discuss how your goal would impact science, technology, and/or society. Focus on what motivates you most about the idea, rather than trying to cover all the impacts. It is better to discuss one impact thoroughly than to try to list all possible impacts.

Evaluation Criteria: I will evaluate the proposals based on writing quality and technical creativity. For writing quality, I am looking for clear, concise technical writing that conveys the ideas of the proposed work. I do not expect a significant number of technical details, since the proposal is very short, and I also do not expect you to have a full understanding of these complex topics since you are not an expert. Instead, I am looking to see that you have a basic grasp of the background materials, and to see what part of the project is most exciting to you, so creativity is encouraged. Note that **you will not be expected to carry out your proposal when you join the group**, but it will give me an idea of what you are most interested in about the project.

Deadline: Please email me the document prior to submitting advisor selection preferences. You may also submit it earlier if you would like to discuss before you submit your advisor selection form.

Background: The brief descriptions of projects and recommended reading are provided below:

- Project 1: Transient kinetic analysis of propane dehydrogenation over oxide catalysts

This project will utilize a combination of transient kinetic measurements, primarily "temporal analysis of products" (TAP), numerical simulations, and machine-learning techniques to understand the kinetic behavior and deactivation mechanism of commercial chromium oxide catalysts used for propane dehydrogenation. This a funded collaboration with Idaho National Labs and Clariant Corporation, who will provide all experimental data. The project is currently funded for 3 years, and has very well-defined objectives and deliverables.

Recommended Reading:
https://linkinghub.elsevier.com/retrieve/pii/S1385894721009657

https://arxiv.org/abs/2011.14473
https://www.sciencedirect.com/science/article/pii/S0021951784711833

- Project 2: Machine learning for electronic structure analysis

This project will utilize the "multipole descriptors" (also called MCSH descriptors) recently developed in our group to accelerate density functional theory (DFT) simulations and/or molecular dynamics simulations. The project will involve working with the SPARC DFT code, and possibly the AMPTorch atomistic machine learning code, and will involve implementation of new techniques in these software packages. The project will be co-advised by Prof. Phanish Suryanarayana from Civil & Environmental Engineering, who is an expert in electronic structure theory, numerical methods, and the lead developer of the SPARC code. The project is currently funded for one year, and there is significant flexibility in the direction.

Recommended Reading:
https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.3.063801
https://arxiv.org/abs/2102.02390
https://arxiv.org/abs/2005.10431

Project 3: Photocatalytic nitrogen fixation (primary advisor: Marta Hatzell)

The main research objective of this project is to enable sustainable point-of-use nutrient production using earth abundant catalysts (minerals), reactants (water, air, wastewater), and renewable energy (sun). Today, nitrogen based nutrient (ammonia) production occurs using an industrial thermo-catalytic fixation process. While effective at producing high yields, this process is far from sustainable, consuming 1-2% of global energy, and emitting 3% of the world's greenhouse gases. This thermo-catalytic process also cannot operate at the small scales required for remote regions, and transportation of nutrients over long distances is often technically and economically not feasible. Therefore, only energy and infrastructure rich countries have access to thermo-catalytic nutrient production. These limitations have contributed to an imbalance in the nitrogen cycle through the emergence of over fertilization in developed countries. At the same time, developing countries suffer from a lack of available nutrients. This project will build on prior work by the Hatzell and Medford group, which focused on farm scale renewable driven production of ammonia using photo and electrocatalysis. In this project, we will focus on designing a high throughput screening apparatus to evaluate viable photoelectrocatalyst for ammonia production. We will also design air breathing electrochemical reactors which allow for combined separations and reactions. Students will gain expertise in electrochemical engineering, reaction engineering, catalysis, energy science, and separations science. Focus will be on experimental investigation, but there will also be the opportunity to perform theoretical and data science analyses to aid experimental efforts.

Recommended Reading:
https://pubs.acs.org/doi/abs/10.1021/acscatal.7b00439
https://pubs.acs.org/doi/abs/10.1021/jacs.8b08464
https://www.cell.com/joule/pdf/S2542-4351(19)30213-2.pdf