

SUMMER 2022 – SC EPSCOR / INBRE RET PROJECT DESCRIPTION FORM

Mentor's Name	Rachel Getman
Institution	Clemson University
Department	Chemical and Biomolecular Engineering
Mailing Address	127 Earle Hall, 206 S. Palmetto Blvd., Clemson, SC 29634
Telephone	864-656-5423
Email	rgetman@g.clemson.edu
Research Subject Area	Computational chemistry

A. Briefly describe overall research program at your laboratory.

My group's research focuses on designing catalysts, which are materials that promote chemical reactions without being consumed or generated during the reactions. There are many types of catalysts. The most common industrial catalyst is probably comprised of nano-sized particles of Pt metal supported on a ceramic or metal oxide material, such as alumina (Al_2O_3). My group and I try to understand the molecular level chemical processes that take place on the surfaces of such catalysts as reactants are converted into products. Specifically, we try to map out the reaction "mechanism," i.e., the "route" from reactants to products, and the thermodynamics (heat of reaction) and kinetics (activation energy) of each step. In doing this, we can make hypotheses about the processes and reaction steps that have the most significant control over the overall conversion from reactants to products. Ultimately, we seek to use this information to design "better" catalyst materials, i.e., materials that are more efficient or less expensive, or which are more "selective" toward production of the most "desired" products, where "desired" products can be more valuable, more environmentally friendly, etc. We currently have projects focusing on catalysts for 1) low temperature production of ammonia, which would help agricultural production in the third world, 2) production of hydrogen gas from glycerol, which would turn something that is produced in surplus into a useful and environmentally friendly fuel, and 3) selective oxidation of alkanes to their primary alcohols, which has applications in both converting natural gas into more valuable energy carriers, as well as general production of fuels from alkanes.

B. Briefly describe specific project(s) for your teacher:

Project 1: This project involves traditional computational catalyst design. Choosing one of the reactions listed above, molecular level models of the reaction mechanism will be developed. Participants will build structures of reaction intermediates on the computer (e.g., using a graphical user interface within a molecular viewer such as the Gaussview software) and use our codes to simulate various aspects of the reaction pathways. They will combine their results with other project team members in order to develop a working hypothesis about how the specific molecules of interest are converted into desired products. This project does not require any coding/programming. It mainly involves chemistry.

Project 2: I have developed a short curriculum on Molecular Aspects of Chemical Engineering targeted at a high school level audience (see <https://lor.instructure.com/?q=rachel%20getman>). Presently the curriculum involves a conceptual overview of quantum mechanics, intermolecular interactions, and an introduction to Monte Carlo. I would like to implement a more in-depth study of Monte Carlo and also an example on machine learning. This work has been started but needs to be made more accessible for high school students. Participants will work with me to upgrade these materials. This project involves some programming in Python; however, no prior coding knowledge is necessary, only a willingness to learn.

- C. Will any other people (post docs, grad students, undergraduate students, colleagues, etc.) be involved directly with your teacher? Most likely yes.**
- D. Will you require any advanced reading/preparation for the teacher? If yes, please briefly describe.** These projects are best suited for people who enjoy computers and chemistry; however, neither project requires any specific computer experience beyond comfort using a laptop/PC to carry out typical tasks such as internet browsing, using spreadsheets or similar software to carry out basic calculations, etc.