

SUMMER 2020 – SC EPSCOR / INBRE RET PROJECT DESCRIPTION FORM

Mentor's Name	Dr. Sapna Sarupria
Institution	Clemson University
Department	Chemical and Biomolecular Engineering
Mailing Address	208 S Palmetto Blvd, Clemson University, Clemson, SC 29634
Telephone	(864) 656-3258
Email	ssarupr@clemson.edu
Research Subject Area	Materials through computational nanoscopes: Discovering materials one molecule at a time!

- A. Briefly describe overall research program at your laboratory.** Sarupria lab focuses on using and developing molecular simulation tools to study materials and processes at the molecular level. Our research falls in the broad theme of computational materials science. Our group focuses on a broad range of problems from ice nucleation in clouds to developing materials for water purification. We study water, polymers and proteins in our group.
- B. Briefly describe specific project(s) for your teacher:** Examples of current projects in our group involve understanding role of surfaces in catalyzing ice nucleation, developing tools to predict the performance of water purification membranes and elucidating the mechanisms through which enzymes can be modified for better stability and activity. During the RET program, the participant will begin with performing some basic molecular simulations. Then the participant will work on a project that is of interest to them based on the broader research themes in our group. For example, a project could include understanding how enzyme interacts with a ligand and developing strategies to mutate the enzyme for better activity. The flexibility of computational modeling allows for the participant to choose a project that most excites them! Simulations are powerful tool to study and visualize the molecular nature of materials. All the software we use in our work is freely available and thus, the participant will be able to use these techniques for teaching and research beyond the project period if they choose to. We will also work with the teacher to incorporate the beautiful visualization of molecular structures and dynamics of the molecules offered through our computational tools into their classes. We look forward to hosting you!
- C. Will any other people (post docs, grad students, undergraduate students, colleagues, etc.) be involved directly with your teacher?** There will be one graduate student that will work directly with the teacher.
- D. Will you require any advanced reading/preparation for the teacher? If yes, please briefly describe.** Some brief reading will be required. Experience with some software will be beneficial (we will provide an easy to follow guide to get you started).