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.

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 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).