SUMMER 2022 – SC EPSCOR / INBRE RET PROJECT DESCRIPTION FORM

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Research Subject Area	Aerosol Formation

A. Briefly describe overall research program at your laboratory:

We use computational chemistry to investigate problems in Atmospheric, Biological, Materials, and Physical Chemistry. Software that solves the mathematical equations for Schrodinger's equation are used to determine the structures and Gibbs free energies for systems of interest. Comparing the structural information graphically with the thermodynamic information allows us to understand the basic chemistry of these systems. Many of our projects allow us to understand the intermolecular forces that are responsible for how groups of molecules interact with each other. So, for instance, six water molecules (a hexamer) in the gas phase form a variety of different shapes, and the lowest energy shapes are the ones that will be found experimentally. The difference between the various hexamers stems from the difference in the hydrogen bonding between these molecules. See (DOI: 10.1126/science.1220574).

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

The biggest uncertainty in Global Warming models is the impact of clouds—will they help cool the Earth or warm it some more? The problem is that clouds are made up of aerosol droplets, and no one really understands how aerosols are formed. Small molecules such as sulfuric acid and ammonia in the atmosphere form pre-nucleation clusters, and at some point these clusters grow large enough to nucleate into an aerosol. We use computational methods to predict the structures and thermodynamics of these clusters, in order to gain insight into how small molecules combine and grow into an aerosol. In our day-to-day work, we submit input to a supercomputer located at Clemson, then after the calculation finishes we examine the output to learn what we can. Besides learning how to use computers to conduct research, a teacher involved in this work would learn the literature for their particular system, and be involved in writing up the results for publication after completion of our work. See (DOI: 10.1021/acs.jpca.1c00872; DOI: 10.1021/acs.jpca.1c05466).

C. Will any other people (post docs, grad students, undergraduate students, colleagues, etc.) be involved directly with your teacher?

One postdoc, one MS graduate student, and 12 undergraduates will all be working in the lab this summer, all of them happy to help our teacher learn the ropes. We can teach you all the technical stuff!