Research Report

AST 287/487 or PHY 287/487

ALL SECTIONS ON THIS FORM MUST BE TYPED EXCEPT FOR THE SIGNATURE SECTION

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AST 287 section #	
AST 487 section #	
PHY 287 section #	
PHY 487 section # 15	
Faculty Name: Marivi Fernandez-Serra	
Semester: (semester and year) (ex: Fall 2017) Spring 2020	

Describe what you actually did this semester. You may wish to mention that you developed problem solving skills, worked independently, worked effectively as a team, developed communication skills, improved knowledge of your discipline, acquired discipline-specific skills.

I worked with Professor Fernandez-Serra. The assigned project was to develop a Python library to analyze the results of atomistic molecular dynamics simulations. In particular the library needed to be written as general as possible. The specific analysis we were aiming for was that of categorizing the atomic species present in the system into super-molecular structures that go beyond the standard chemical nomenclature. These super-molecular structures have their own hierarchy of complexity or category. The project involved identifying the categories and their lineage. This process requires a deep understanding of the material physics and chemistry because it necessary to identify when an atom or group of atoms belong to different system parts. This identification is done in terms of bond lengths, with cut offs, values that depend on the particular category. Since these categories are not standard I had to determine all these parameters on my own. Although the library structure is designed to be as general as possible the categories I programmed were designed to identify different forms of water-related oxygen atoms that occur at the interface of a perovskite oxide material with liquid water. Hence, my classification programs needed to identify surface molecular waters, bulk molecular waters, surface hydroxyls, bulk hydroxyls, surface hydroniums, bulk hydroniums, etc. Additionally, the research allowed me, in general, to gain a valuable experience with the powerful programming language that is Python. In utilizing many of its unique capabilities to perform this complex data analysis, I gained a complete introductory course's worth of knowledge of the language up to the more advanced topics of object-oriented programming, inheritance, and abstract classes. This was an excellent opportunity which allowed me develop my coding skills, learn a new language, and do all this while learning to complete these tasks on a mostly independent basis.

Are you going to present a poster on your work? No

Signature Section:	
Student Signature Steven Paci	Date: 5/5/2020
Faculty Signature	Date: 5/5/2020
Undergraduate Director Signature	Date: 5/5/2020