



AST 287/487 or PHY 287/487 Research Registration

As opportunity for selected undergraduates to conduct faculty-supervised research for academic credit. Research proposals must be prepared by the student and submitted for approval by the supervising faculty before beginning the credit period. An account of the work and results achieved is submitted to the supervising faculty before the end of the credit period. May be repeated for up to a total of three credits for AST/PHY 287 and six credits for AST/PHY 487.

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

Student Name: Steven Paci Jr.	Student I.D. #: 108980329
Email address: steven.paci@stonybrook.edu	
AST 287 section #	
AST 487 section #	
PHY 287 section #	
PHY 487 section # 15	
Faculty Name: Marivi Fernandz-Serra	
Credits to be earned: 1 credit = 4 hours work per week3	
Semester: (semester and year) (ex: Fall 2017)Spring 2020	
<p>Describe research project to be completed this semester:</p> <p>Developing a Python Code to identify “ super atomic ” species:</p> <p>When water interacts with surfaces, it can dissociate. It can also behave in different ways to its natural bulk behavior. Either enhancing its hydrogen bonding ability or decreasing it. A water molecule at a given surface might not be identifiable as a highly reactive species based only on its structural and environmental variables. It can actually be electronically correlated to nearby molecules or to the nearby surface. Identifying specific electronic motives which might indicate which atomic species are correlated or which atoms are chemically different despite belong to the same species is not a trivial problem. In this project, the student will develop a code to analyze molecular dynamics simulations of water in different semiconductor surfaces. This code will be able to characterize the atoms beyond their regular molecular environments, constructing new “ super-atomic” species capable of characterizing the reactivity of the underlying semiconductor surface.</p>	
<p>Please note: Students enrolled in PHY 287 or 487 or AST 287 or 487 are expected to present their work at the annual URECA celebration.</p>	
<p>** Research Report must be completed just prior to the end of the semester**</p>	
Signature section:	
Student Signature : 	Date:01/30/2020
Faculty Signature : 	Date:01/30/2020
Undergraduate Director Signature:	Date:01/30/2020