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Undergraduate Research Program	
Project Name	Coarse-grained modeling of chocolate fat bloom formation for molecular dynamics
Campus & Location in Mexico	Querétaro
Faculty	Engineering
Research Area	Nanotechnology for Device Design
Research Responsible	Claudia Elena Ferreiro Cordova
Description of the Project	Chocolate bars, such as the ones that can be found easily in supermarkets, are in a metastable state that can be perturbed under temperature fluctuations, which are not unusual for commercial chocolate bars. Under such conditions, chocolate will undergo phase separation and darker and lighter color regions will appear. These regions correspond to regions that are reachier in fat or have less fat than the original chocolate bar. In this project the student will work on the development of an appropriate coarse- grained for cocoa butter that could be applied to computer simulations using molecular dynamics. This project focuses on defining an appropriate interaction model for such molecules that can allow us to study the phase instabilities common to commercial chocolate bars. The aim is to start tackling a theoretical model for cocoa butter molecules that will allow us to make predictions, and that can also be implemented in molecular simulations. This project will include: 1 Research of the theoretical framework. 2 Proposal of model. 3 Cluster formation of cocoa butter molecules, as a way to study phase separation. 4 Preliminar molecular simulation runs.
	framework;Scientific-based problem solving
Modality	Hybrid
Offered During	Winter (5 weeks)

Student		
Tasks/Responsibilities	 -Literature review of the subject. -carry on calculations To validate the model. -carry on trial simulations To test cluster formation. 	
Required Language Proficiency	Spanish (Medium);English (Medium)	
Required Skills and Abilities	Basis of statistical mechanics and thermodynamics.	
Other Documents Required to APPLY for an Internship	 Being at least in your 2nd year of bachelor Accumulative grade point average (GPA) 2.5 Official Transcript 2 letters of recommendation of faculty members Resume Letter of intention explaining the reason why you would like to participate in the research program 	