Introduction
A primary goal of dental research is to prevent tooth decay, principally by stopping formation of plaque, which is a film composed of bacteria. To help prevent tooth decay, more information about the chemical interactions present between substances in the saliva and the tooth enamel is needed. An integral component within this system is the dental pellicle, the protective layer between the tooth enamel and saliva. The pellicle is composed of proteins, carbohydrates and lipids; however, the precise structure and composition is unknown. The exact details of the interactions between the pellicle and the enamel is currently unknown, but this study is a vital first step in understanding what is happening at the tooth’s surface. The thought was that building a model of the pellicle with the mineral layer of enamel, hydroxyapatite, could be the first step towards understanding interactions between the pellicle and enamel.

Proteomics studies have been done on the composition of the pellicle, but few show the interactions between ionic substances within the layer and the hydroxyapatite-Ca$_3$(PO$_4$)$_2$·OH. This construction was done by computationally modeling the various components in the pellicle.

Building Pellicle Model
One goal of the project was to construct the first atomic model of the pellicle. Macromolecules of the pellicle were found through literature searches of proteomics, lipid, and carbohydrate composition studies. We integrated these into an all-atom structure of the pellicle was generated by compiling these compositions with the accepted thickness and density of the new pellicle after two hours (Reference 17 on Word). The numbers of each molecule type included in our pellicle model are based on a density of 0.5 g/ml which is consistent with experimental data.

The structure of the enamel is derived from the crystal structure of hydroxyapatite, was determined to be made up of hydroxyapatite through many sources (References). The hydroxyapatite picture was then generated.

Pellicle
Pellicle- composed of proteins (gray), carbohydrates (green), and lipids (blue)

Plaque Formation
Plaque forms when bacteria, usually Streptococcus mutans, in the pellicle make glucans from carbohydrates in the pellicle. Excess sugar, especially sucrose, may lead to excess plaque buildup if not properly treated. The sugar can be used as an easy way for bacteria to synthesize glucans. A lesser sugar intake has been suggested to prevent bacterial buildup. This aggregation of bacteria leads to biofilms, which are colonies of bacteria that can exist anywhere in a person’s body and are difficult to break up. Dental biofilms, or plaques, occur when a person does not brush off the pellicle for a period of time. Regular brushing of a couple of times per day does not adequately remove the pellicle. The poor removal of the pellicle gives the bacteria time to form a larger biofilm, creating plaque that may only be able to be removed through dental cleanings. If plaque is left untreated, bacterial proteases likely will breakdown proteins in the pellicle and the layer itself, exposing enamel. Acid by-products of bacterial metabolism will eventually lead to enamel degradation. This is a direct cause of cavities, or carries, that may lead to even more serious oral health problems.

Enamel
Hydroxyapatite composed of phosphate(phosphorus-ochre), calcium (cyan), and hydroxide (oxygen-red)

Fluoride Versus Hydroxide
Fluoride has been shown to be successful in preventing dental caries. A second goal of this project was to examine the mechanism by which fluoride can protect the tooth from demineralization. Crystals of hydroxyapatite and fluoroapatite were simulated in a solution containing glucose molecules in order to determine whether the substitution of fluoride for hydroxide ions in tooth enamel alters the binding of glucose. To measure association of glucose with enamel, radial distribution functions (RDFs) between phosphorus atoms in the enamel and glucose were calculated from the simulations. The radial distribution function, which is a measure of the probability of finding two groups within a given separation of each other, were then used to calculate the Gibb’s free energy, which is a measure of the strength of interaction between glucose and the enamel surface.

Gibb’s Free Energy $\Delta G = (-) RT \ln (RDF)$

Discussion
From this work we built the first all-atom model of the dental pellicle. We did this in order to better examine the pellicle composition and give other researchers a better representation of this important biological structure. Future research can use this model to give a visual representation for their research and for people they may be explaining it to. This visual aid is simple enough to allow for people unaware of the pellicle’s existence to better understand what it is composed of and the possible interactions that may take place.

The fluoroapatite versus hydroxyapatite project allows for an understanding of the physical properties of each substance and their relations to glucose. This can serve as a framework for research dealing with bacterial adhesion to both types of enamel surfaces.