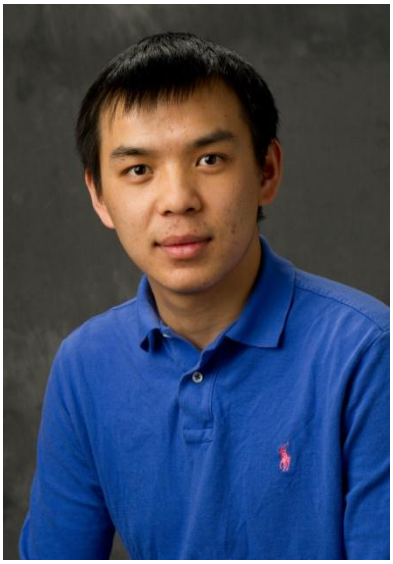

Hector Chang received his B.S. degree in Agricultural and Biological Engineering (2009) in the field of Biological and Food Processing Engineering from Purdue University. During his undergraduate studies, he worked with Dr. Campanella in rheological studies of refrigerated dough. He decided to purdue a M.S degree in the same department under Dr. Narsimhan to study the conformation changes of antimicrobial peptide on silica surface using molecular dynamics simulation and circular dichroism.

Agricultural & Biological ENGINEERING

Thesis Defense

Speaker: Hector Chang

Title: Conformational Changes of an Antimicrobial Peptide "Cecropin P1 on Silica Surface: Molecular Dynamics and Circular Dichroism Studies

Major Professor(s): Dr. Narsimhan

Date: Friday, June 01, 2012

Time: 2:30 PM

Location: ABE 301

Abstract:

Antimicrobial peptides (AMP) are innate mechanism of defense of the immune system found in insects and animals. It is shown that these peptides act against pathogenic bacteria, fungi, enveloped viruses, parasites and cancerous cells. Our objective in this project is to investigate the conformational changes of an AMP, namely, Cecropin P1 (CP1) on silica surface by using molecular dynamics (MD) simulation and circular dichroism (CD). It is important to study the protein structure CP1 on silica surface to determine the secondary structure changes due to immobilization. The secondary structure of CP1, α-helix, is an important factor for their antimicrobial activity mechanism (cell membrane disruption) . Explicit solvent MD simulation of five Cecropin P1 C molecules tethered to cosite silica with (Poly ethylene oxide)$_3$ linker for two different peptide-peptide distances of separation (3 nm and 5 nm) indicated that the total α helical content was lower for larger distance of separation as a result of reduced peptide-peptide interaction. Hydrophobic solvent 2-2-2 trifluoroethanol (TFE) was found to increase α helical content of Cecropin P1. Overall, the results from MD and CD showed a reduction in α-helix content when CP1 is immobilized on silica surface.

Application:

This research will provide a new alternative for antibiotics where bacteria are unlikely to develop resistance against antimicrobial peptides. It will be a good application for food packaging or any applications related to the prevention of harmful bacteria.