ST. FRANCIS XAVIER UNIVERSITY

Physics Colloquium

Friday, 8 January 2010, 4:00pm, PSC 3046

Jeremy Thorbahn

Modeling a Stealth Delivery Vehicle for Antimicrobial Peptides

Gram-Negative bacteria such as E. Coli and Salmonella are well known as food-borne pathogens. Hence, the ability to eliminate these harmful agents is very important in the advancement of food preparation and preservation technologies. Experiment has shown that certain cationic antimicrobial peptides (CAPs) are able to destroy Gram-Negative bacteria if the peptides have access to the bacterial surface. Protamine, the CAP we will be studying, has many positively-charged amino acids which leave it vulnerable to the influence of charged food proteins and polysaccharides before it ever reaches a bacterial surface. Therefore, an effective means of delivering protamine to destroy bacteria within a food requires a shielded vehicle which can contain the peptides until they reach their target. Using Monte Carlo simulation, we will model this delivery vehicle and examine its ability to effectively deliver protamine to the surface of Gram-Negative bacteria.

Megan Cuthbertson

Local Order Parameters in a Liquid-Liquid Phase Transition of Water

Water is one of the most important and ubiquitous materials in science as well as in everyday life. Despite being so common, it remains mysterious in many ways. Experiments have demonstrated the existence of two distinct phases of solid amorphous (glassy) water: high density amorphous (HDA) ice and low density amorphous (LDA) ice. An unresolved question is whether or not this same phenomenon is seen in liquid water. That is, do two distinct phases of liquid water occur in the supercooled regime? Using molecular dynamics simulations of the ST2 model of water, we investigate the properties of high density and low density liquid water. In general, thermodynamic phases are distinguished by order parameters. In this case, we use the local density, related to the distance of the 5th neighbour molecule, to differentiate the two phases of liquid water in our simulations, and then study these phases under a variety of temperature and density conditions.