

**Name:** Robert (Robbie) Leske

**Year in Course:** 2nd (Junior)

**Topic:** Physical Chemistry, Quantum Biology, Chemical Simulations

**Mentor:** Dr. Raymond Kapral, University of Toronto; Dr. Dennis Salahub and graduate students, University of Calgary

**Title:** A Combined Quantum Mechanics and Molecular Mechanics Simulation of the Chlorophyll Complex Involved in Photosynthesis

**Abstract:**

Photosynthesis is the process through which plants and other autotrophs harvest light energy from the sun and convert it to chemical energy for use later. However, the process is unusually efficient and has astounded scientists for years. It is currently believed that plants make use of superposition for electrons to travel every possible path at the same time allowing the electron to find the most efficient pathway. However, this raises the question how plants can avoid decoherence: the collapse of the wave function through interaction with the environment. This research will use a combined quantum mechanics and molecular mechanics (QM/MM) simulation of a photosynthetic system in order to provide more information to the field of quantum biology. We anticipate accurate results based on similar previous studies. We hope that the results from this study will help to determine whether the effects of vibration, electronic interactions, or a combination is the reason for coherence in plants. An understanding of this phenomena could be applied to quantum computers in order to avoid decoherence at higher temperatures with less expensive equipment.