

The Summer Research Project -- Project Proposal

Form 1

Summer student research opportunities are available and sponsored by NSERC as Undergraduate Summer Research Awards (USRA) or as part of the financial need-based award program provided by the University of Guelph known as the Undergraduate Research Assistantships (URA)	
Department: <p style="text-align: center;">Chemistry</p>	Name and Title of Proposed Supervisor: <p style="text-align: center;">Dr. John D. Goddard, Professor</p>
Proposed Starting Date: May 05, 2008	Application:
Title of Proposed Research Project: <p>Density Functional Theory for the Prediction of Structural and Spectroscopic Properties of Perfluoro-alkanes.</p>	URA X or USRA X
<p>Completely fluorinated organic compounds such as perfluorooctanes and their derivatives for example perfluorooctane sulfonates (PFOS) show remarkable chemical properties. For example, longer chains adopt intriguing helical structures very different from the geometries of ordinary hydrocarbons. We are using several theoretical models to better understand the origin of these structural preferences. We predict the NMR spectra of the molecules as ¹⁹F NMR is widely used to identify and characterize these compounds. Using computational chemistry software such as GaussView and Gaussian03, the summer research student will model long chain perfluoroalkanes. <i>Ab initio</i> Hartree-Fock and Møller-Plesset models will be used to complement density functional schemes in the prediction of the relative energies, the geometries, the vibrational frequencies, and the NMR spectra for a large database of perfluoro-alkanes. The accuracy of a number of the most modern exchange correlation functionals will be examined. Extensive use will be made of Windows and Linux based computers in the computational quantum chemistry laboratory as well as the SHARCnet high performance computing facilities.</p>	
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Signature of Proposed Supervisor : _____ Signature of Chair of Department: _____ Printed Name of Chair of Department: Prof. Adrian Schwan Date: December 20, 2007	

