

**M.Sc. Defense**  
**Bayden Pritchard**  
**DATE: Monday December 13<sup>th</sup>, 2010**  
**TIME: 9:30a.m.**  
**PLACE: Science Complex 1511**  
**University of Guelph**

**THESIS TITLE:**

Optimized Pair Distribution Function Analysis of Gold Nanoparticles

**ABSTRACT:**

A fast and efficient method for creating quantitative pair distribution functions (PDFs) was developed for use on a range of sample types. A volume correction was modelled in parallel with work on an optimized PDF calculation method. It was shown that the optimized calculation method eliminated the need for specific physical corrections which otherwise contaminate PDFs, thus greatly improving the efficiency of PDF calculation. Proof of this principle and of the PDF's quantitative accuracy was demonstrated using a standard sample, bulk gold. To demonstrate the versatility and power of the new PDF analysis method, non standard samples consisting of gold nanoparticles of various sizes were analyzed. For the first time, properties such as thermal expansion, lattice constant and Debye-Waller factors of these nanoparticles were measured via the optimized PDF method and are presented here.

**EXAMINING COMMITTEE:**

**Chair: Dr. Robert Wickham**

**Advisor: Dr. Stefan Kycia**

**Advisory Committee Member: Dr. DeTong Jiang**