

**Workshop: Quantum Chemical Computations in NMR**

Tuesday, December 18, 2007, 1200 Montreal road, M-40

Organized by:            **University of Ottawa**  
                                 **SIMS National Research Council Canada**  
Hosted by:             **National Ultrahigh Field NMR Facility for Solids**

**Workshop program:**

- 13:00-13:15**    Welcome
- 13:15-14:15**    Keynote lecture, **Tom Woo** (University of Ottawa) "A Practical Introduction to Solid State DFT Calculations with Periodic Boundary Conditions and Plane Wave Basis Sets"
- 14:15-14:35**    **Igor Moudrakovski** (NRC-SIMS) "NMR parameters in small inorganics with CASTEP: first impressions"
- 14:35-14:55**    **David Bryce** (University of Ottawa) "Comparison of experimental Ca-43 and Cl-35/37 quadrupolar and chemical shift tensors with those obtained from CASTEP"
- 15:00-15:15**    Coffee Break
- 15:15-15:40**    **Darren Brouwer** (NRC-SIMS) "Refinement of crystal structures using ab initio calculations of NMR parameters"
- 15:40-16:05**    **Saman Alavi** (University of Ottawa) "Computation of NMR lineshape anisotropies of guest molecules in inclusion compounds: CO<sub>2</sub> in large structure I clathrate cages"
- 16:05-16:30**    Closing discussion, coffee, tour of the NMR Facilities at M-40

**Keynote lecture, Tom Woo (University of Ottawa)**

"A Practical Introduction to Solid State DFT Calculations with Periodic Boundary Conditions and Plane Wave Basis Sets"

**Abstract:** Performing molecular DFT calculations with Gaussian basis sets is now common place. However, solid state DFT calculations of periodic systems are often performed with very different technologies. For example, so-called plane wave basis sets or similar are often used. The current state-of-the art solid state NMR calculations with the CASTEP or CPMD packages use these technologies. In this tutorial, an introduction to solid state DFT calculations will be given. No back ground in solid state physics will be assumed, and there will be an emphasis on the practical aspects of performing such calculations.