

**Joint Seminar Series of the  
CENTRE FOR RESEARCH IN MOLECULAR MODELING  
and the DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**

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***Quantum Molecular Dynamics of  
Molecules Embedded in Complex Environments***

We will present approaches for the theoretical study of molecular dynamics in complex environments such as superfluid clusters and nano cages. We will mostly focus on path integral simulation techniques and will consider both atomic and molecular bosons as the constituent of the superfluid. We will show that the superfluid response to the rotational dynamics of a molecule can be used to explain microwave and infrared spectroscopic experiments [1,2]. We will discuss the challenges associated with different types of rigid tops [3]. Results will be presented for the case of asymmetric top molecules trapped in parahydrogen clusters and the idea of a genuine probe of superfluid response will be introduced [4]. Recent results for quantum rotors trapped in water cages will be discussed. A perspective on future challenges including the study of quantum dynamics in flexible polyatomic molecules will be presented.

**References**

1. H Li, R. J. Le Roy, P.-N. Roy, A.R.W. McKellar, Phys. Rev. Lett. 105, 133401 (2010).
2. P. L. Raston, W. Jäger, H. Li, R. J. Le Roy, and P.-N. Roy Phys. Rev. Lett. 108, 253402 (2012).
3. T. Zeng, H. Li, and P.-N. Roy, J. Phys. Chem. Lett. 4, 18 (2013).
4. T. Zeng, G. Guillon, J. T. Cantin, and P.-N. Roy, J. Phys. Chem. Lett. 4 239 (2013).



**Pierre-Nicholas Roy** received his bachelor degree in chemistry from McGill University in 1990. He then pursued graduate studies in theoretical chemistry at Université de Montréal where he received his M.Sc. in 1993 and his Ph.D. in 1997. He spent the year 1997 at the James Franck Institute of the University of Chicago as a Research Associate. He then moved to the University of Utah in 1998 as a Postdoctoral Fellow in the Henry Eyring Institute for Theoretical Chemistry. He returned to Canada in 1999 to join the University of Alberta where he was Assistant and Associate Professor of chemistry until 2008. He moved to the University of Waterloo in 2008 where he is a Professor of Chemistry and holds a University Research Chair. In the year 2000, Pierre-Nicholas Roy received the Research Innovation Award from the Research Corporation. He also received the 2007 Keith Laidler Award from the Canadian Society for Chemistry. His group is involved in the development of new theoretical and computational methods to simulate the quantum dynamics of complex molecular systems.