Centre for Research in Molecular Modeling
CERMM
Centre de recherche en modélisation moléculaire

UNIVERSITÉ Concordia UNIVERSITY

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

April 9, 2014, 2:30 PM – SP-265.29

Christopher Rowley
Memorial University of Newfoundland

Multiscale Computational Chemistry

Our research group uses computer modeling to understand complex chemical processes. These processes can occur on length scales spanning from the picometer to the nanometer and time scales that span from the femtosecond to the microsecond, so we use special computational methods capable of describing systems that span these scales. In this talk, I will present three applications of these methods by our group. In the first example, we use polarizable molecular dynamics simulations to identify why the toxic gas hydrogen sulfide is able to permeate across cell membranes but water is not [1]. We have also used replica-exchange molecular dynamics and a coarse grain protein model to help elucidate the structure of a protein linked to a genetic disease. In the third example, we use the CHARMM-TURBOMOLE QM/MM program developed in our group [2] to determine why Zn(II) is more soluble in water than Mg(II), despite the fact that the ion-water distances are the same for both ions [3].

[1] Riahi, S., Rowley, C.N. *J. Am. Chem. Soc.* **2014**, DOI: 10.1021/ja508063s
[2] Riahi, S., Rowley, C.N. *J. Comput. Chem*. **2014**, DOI: 10.1002/jcc.23716
[3] Riahi, S., Roux, B., Rowley, C.N. *Can. J. Chem.* **2013**, DOI: 10.1139/cjc-2012-0515

Christopher Rowley was born and raised in Ottawa, the national capital of Canada. I completed my undergraduate degree in computational chemistry at Carleton University in 2004. I completed my Ph.D. in 2009 at University of Ottawa with Professor Tom Woo. I held an NSERC Postdoctoral Fellowship at the University of Chicago in the Department of Molecular Biology and Biochemistry with Professor Benoît Roux. I joined the Department of Chemistry at Memorial as an Assistant Professor in January, 2012.