

**Joint Seminar Series of the
DEPARTMENT OF CHEMICAL AND MATERIALS ENGINEERING and the CENTRE FOR
RESEARCH IN MOLECULAR MODELING**

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Molecular Simulation – an Enabling Tool for Research

Undoubtedly, the ultimate goal of many branches of science is to achieve a complete understanding of the correlations between molecular behaviour and the corresponding observed properties of systems that are made up of such molecules. From an industrial perspective, such understanding will definitely help scientists and engineers design materials and the associated manufacturing processes more efficiently. With advances in computer technology and developments in molecular simulation methods over the past few decades, complex molecular systems can now be readily investigated. In fact, such simulation methods provide an effective means to study how do molecular structure and atomic-level interactions determine macroscopic properties of materials of interest as well as how do these materials response to the imposed processing conditions, information that is difficult to obtain experimentally. In this seminar, I will present some selected research problems that my group has encountered over the past couple decades to illustrate how molecular simulation has been applied to further our understanding of the systems of interest. These research problems include non-equilibrium nanoflow, design of collectors for minerals processing, CO₂ capture using hydrotalcites-derived mixed oxides, macromolecular drug delivery systems and permeability of food packaging materials. Finally, I will finish up the seminar with our most recent results on the study of the diffusion of unentangled polymer melts using a non-linear Brownian dynamics model.



Phillip Choi is Professor of the Department of Chemical and Materials Engineering at the University of Alberta and is a registered professional engineer in the province of Alberta and a Fellow of the Chemical Institute of Canada. Prof. Choi is also an active consultant to various multinational organizations on issues related to polymer products development and polymer failure analysis. He received his BSc (1988) in chemical engineering from the University of British Columbia and his MSc (1992) and PhD (1995) from the University of Waterloo. During the period of 1990 – 1995, he was a visiting scientist at Xerox Research Centre of Canada. His current research interests lie in the areas of design/development of synthetic and bio-based polymers for applications involving controlled release of small molecules and of solvent extraction of oil sands, respectively. He has authored and co-authored 3 book chapters, 116 referred journal publications and 1 US patent. He is also a coauthor of a textbook entitled “The Elements of Polymer Science and Engineering,” 3rd edition (2013) published by Elsevier. Prof. Choi was named the McCalla Professorship in 2007 and won the Faculty of Engineering Undergraduate Teaching Award in 2008 at the University of Alberta recognizing his dedication to undergraduate education. He received a National Young Innovator Award from Petro Canada Inc. in 2001 and an international IUPAC Travel Award in 2002, respectively, recognizing his work on polymer research.