

## SEMINAR

You are invited to attend the Graduate School of Biomedical Engineering seminar:

### ATOMIC SCALE SIMULATIONS TO ADVANCE OUR UNDERSTANDING OF GENE AND DRUG DELIVERY

#### Prof Sean Smith

Professor in Computational Nanomaterials Science and Engineering  
Director, Integrated Materials Design Centre (IMDC)  
School of Chemical Engineering  
UNSW Australia



12 pm, Friday, September 25, 2015

Seminar Rm (513), level 5, Samuels Building, UNSW

*Lunch will be served following the talk.*

**Abstract:** Recent advances in synthetic polymer chemistry have provided a wealth of complex polymer architectures such as comb polymers, star polymers and amino acid dendrimers that have interesting chemical, solution, melt, adsorption and mechanical properties and offer many new opportunities for enabling drug and gene delivery. There is however a substantial knowledge deficit on the supramolecular structures that are created when drugs are complexed with these carrier, or vector, architectures. This knowledge gap inhibits the rational design and optimisation of new therapeutic agents.

In this programme of work, the new UNSW Integrated Materials Design Centre develops atomic-scale models using molecular mechanics and molecular dynamics codes to predict the structures, stabilities and dynamics of drug-vector complexes. The predicted structures are verified against analytical methods including small-angle neutron scattering and small-angle X-ray scattering. The end game is to develop new insights for co-design of drugs and vectors based on pharmaceutical delivery efficiency in order to enhance the power of nanomedicine.

**Bio:** Sean Smith received his PhD in theoretical chemistry at the University of Canterbury, New Zealand, in 1989. Following an Alexander von Humboldt Fellowship at the University of Göttingen and postdoctoral research at the University of California, Berkeley, he accepted a faculty position at The University of Queensland, Australia in 1993. He became Professor and Director of the Centre for Computational Molecular Science at UQ in 2002 and in 2006 his laboratory moved to the Australian Institute for Bioengineering and Nanotechnology at UQ. He worked with colleagues in the ARC Center of Excellence for Functional Nanomaterials 2002-2011 as Program Leader (Computational Nanoscience) and Deputy Director (Internationalisation). In 2011, he accepted the position of Director of the US Department of Energy funded Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory, one of five major DOE nanoscience research and user facilities in the US. He joined the School of Chemical Engineering at UNSW Australia in 2014. His specific research involves theoretical and computational studies of chemical kinetics; reaction dynamics; catalysis; as well as structure, self-assembly and transport phenomena within nanomaterials, proteins, and hybrid nano-bio systems. He has published over 230 refereed journal papers. In 1998 he was elected Fellow of the RACI. In 2006 he was recipient of a Bessel Research Award of the Alexander von Humboldt Foundation in Germany and in 2012 he was elected Fellow of the American Association for the Advancement of Science (AAAS).