

DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2018

DATE: TUESDAY, FEBRUARY 6, 2018

**WHERE: ELECTRICAL AND COMPUTING ENGINEERING
DEPARTMENT - 202**

TIME: 10:00 AM

GUEST SPEAKER

Dr. Sergei Manzhos

Assistant Professor

Department of Mechanical Engineering

National University of Singapore

Singapore

TOPIC

Computational materials modelling and design for next generation energy conversion and storage technologies: practical design strategies and improved methods

ABSTRACT

I will present recent results and ongoing work on ab initio modelling and design of materials, focusing on materials for next generation electrochemical batteries and solar cells. Specifically, I will present comparative studies of intercalation of ions differing by ion size (e.g. Li vs Na vs K) and valence (e.g. Li vs Mg vs Al) in different phases of several prospective active electrode materials including carbon, Si, Sn, TiO₂ and vanadium oxides, as well as studies of organic electrode materials. I will show how ab initio modelling can help develop efficient strategies to improve voltages or enable electrochemical activity for post-lithium storage. I will also dwell on methodology issues one has to deal with when modelling battery materials such as treatment of vdW interactions or deficiencies of functionals or construction of amorphous phases.

I will then present our recent results in modelling of electron and hole transport layers for perovskite solar cells and show how molecular modelling can help resolve these important bottlenecks on way to commercialization of this type of cells. I will highlight the importance of aggregate state modelling of these materials for calculation of electron/hole transport rates and optical properties, arising methodology issues, and how we have dealt with them.

At the end of the talk I will give a brief summary of my work addressing some of the limitations of workhorse modelling methods: large-scale ab initio modelling with Orbital-free DFT and anharmonic vibrational spectroscopy suitable for interfaces.

BIOGRAPHY

Sergei Manzhos is Assistant Professor at the Department of Mechanical Engineering, National University of Singapore. He works on computational materials modelling and design, specifically for applications in advanced electrochemical batteries, focusing on post-lithium and organic batteries, and advanced solar cells, focusing in charge transport materials for perovskite solar cells. Dr. Manzhos is also active in method development in the areas of quantum dynamics (computational vibrational spectroscopy and potential energy surfaces) and large-scale ab initio methods (Orbital-free DFT). He hold PhD in chemistry from Queen's University, Canada (2005) and prior to NUS worked as NSERC Postdoctoral Fellow at the University of Montreal, Canada (2005-2008) and Project Assistant Professor at the University of Tokyo, Japan (2008-2012).

Committee members:

Dr. Lev Krasnoperov, Dr. Alexei Khalizov, Dr. Yong Yan