NUS Department of Mechanical Engineering

The Mechanical Engineering Department cordially invites you to our:

DEPARTMENT SEMINAR

Topic:	**Computational Modeling of Molecule-Surface Interactions for Sustainable Energy Schemes**
Speaker:	**Dr Sergei Manzhos** *Assistant Professor, Research Centre for Advanced Science & Technology (RCAST), University of Tokyo, Japan*
Date:	**Tuesday, 22 November 2011**
Time:	**11:15 am –12:30 pm**
Venue:	**EA-06-04** *(map of NUS can be found at http://www.nus.edu.sg/campusmap/)*

Abstract

In the search for new and cleaner energy sources, a central role is played by molecule-surface interactions. Examples range from catalyzed production of H_2 for fuel cell applications to the conversion of solar into electrical energy. The speaker will first discuss tools they have developed to: (i) predict the dynamics of molecule-surface reactions using continuous potential energy surfaces (PES); and (ii) compute anharmonic vibrational spectra of molecules on surfaces. PESs for polyatomic molecules on surfaces are unavailable today, which forces researchers to compute only static potential diagrams or to use expensive direct ab initio dynamics to predict reaction outcomes. A general method to build such PESs based on neural networks and dimensionality reduction[1] and a recent application to N_2O on Cu, will be presented. Ability to compute IR spectra is essential for species identification. A method to compute anharmonic spectra directly from ab initio data[2], has been developed. Application to H_2O on Pt will be shown. The speaker will then focus on dye-sensitized solar cells (DSSC). DSSCs have the potential to become an economical solar energy conversion technology. They are obtained by sensitizing a semiconductor with a dye molecule that absorbs visible light and injects electrons from its excited state into the conduction band of the semiconductor. The dye is then regenerated by an electrolyte. DSSCs have reached an efficiency of over 11%. Further efficiency gains require a deeper understanding of the relation between molecular and molecule-semiconductor-electrolyte structure and the conversion efficiency. Computational models that relate dye structure to injection and recombination via non-adiabatic coupling constants[3], will be presented. Applications to solar cells operating by interfacial charge transfer bands using catechol-thiophenes and TCNE, TCNQ, TCNAQ will be shown. The speaker will also present their recent and ongoing studies of the effect of nuclear motion on injection in DSSCs and of the behavior of computational errors in the calculations of absorption spectra of organic dyes differing by conjugation sequence.

1 S. Manzhos, K. Yamashita, T. Carrington Jr., Comp. Phys. Comm. 180 (2009) 2002; S. Manzhos, K. Yamashita, Surf. Sci. 604 (2010) 555.
2 S. Manzhos, K. Yamashita, T. Carrington, Chem. Phys. Lett. 511 (2011) 434; Surf. Sci. 605 (2011) 616
3 S. Manzhos, H. Segawa, K. Yamashita, Chem. Phys. Lett. 501 (2011) 580; ibid. 504 (2011) 230; S. Manzhos et al., J. Phys. Chem. C (2011) DOI: 10.1021/jp205187a

About the Speaker

Dr Sergei Manzhos received a M.Sc. from Kharkiv National University, Ukraine, in 1999 and a Ph.D. from Queen's University, Canada, in 2004, under the supervision of Prof Hans-Peter Loock. He was a Postdoctoral Fellow at the University of Montreal with Prof Tucker Carrington from 2005–2007 and an Assistant Professor at the Department of Chemical System Engineering, University of Tokyo, from 2008–2009. Since 2010, he has been an Assistant Professor at RCAST, University of Tokyo, Japan. Research interests include theory of molecule–surface reactions and of dye-sensitized solar cells as well as theoretical spectroscopy with the focus on molecule-surface complexes.

****Admission is Free. All are welcome to attend.****