Chemical and Petroleum Engineering

SEMINAR NOTICE

Michael Eikerling

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Prof. Michael Eikerling assumed his faculty position at Simon Fraser University in May 2003 and he was promoted to the rank of Full Professor in 2012. He received his Diploma in theoretical condensed matter physics from RWTH Aachen University in 1995 and obtained his doctoral degree from TU München in 1999 with thesis on the theory of fuel cells. Prior to joining SFU, he spent periods as a research associate at Research Center Jülich (9/1998 to 8/2000), Los Alamos National Laboratory (9/2000 to 2/2002), and TU München (2/2002 to 4/2003). From 2003 to 2006, he held a Provincial Research Fellowship in Fuel Cell Technology from the British Columbia Innovation Council. From 2003 to 2013, he was cross-appointed to the National Research Council Canada-Institute for Fuel Cell Innovation, Vancouver, where he shaped activities in physical modeling of electrochemical energy materials.

The group of Prof. Eikerling harnesses a wide spectrum of physical methods, from quantum mechanical simulations and molecular modeling to non-equilibrium thermodynamics, condensed matter theory, and statistical and continuum theories of heterogeneous media. Research interests in the group span a diverse range from fundamental to applied topics, encompassing molecular modeling of self-organization in electrochemical materials; theoretical electrocatalysis; modeling transport and reaction at interfaces and in nanoporous media; statistical physics of heterogeneous media; porous electrode theory; electrochemcal diagnostics; and performance and degradation modeling of electrochemical devices. He has published > 120 papers (h-index: 36, > 4,000 citations), published a textbook on Polymer Electrolyte Fuel Cells in 2014, serves the electrochemical community in various leadership roles, and trained > 20 HQP since 2011 (11 currently). In 2017, he was awarded the Alexander Kuznetsov Prize for Theoretical Electrochemistry of the International Society of Electrochemistry.

"Hierarchical Modeling of Catalyst Layers in Polymer Electrolyte Fuel Cells"

Abstract

The ever-escalating demand for efficient and environmentally benign energy technologies drives research on electrochemical materials and systems. In this realm, theory, modeling, and simulation contribute increasingly powerful methods and tools to study how complex multifunctional materials come to life during self-organization, how they live and function, and how they age and fail because of wear and tear during operational life. After providing a sweeping overview of research activities in this field, the presentation will focus on frontier-type topics in theoretical electrocatalysis and modeling of catalyst layers for polymer electrolyte fuel cells. First, a theoretical framework for deciphering the oxygen reduction reaction will be presented [1]. It combines microscopic information on reaction mechanisms and pathways, obtained from density functional theory simulations, with a recently developed model of the non-monotonic surface charging relation of platinum [2,3]. Next, the role of ionomer incorporation for local reaction conditions and transport phenomena in catalyst layers will be discussed [4,5,6]. In the final part, macrohomogeneous catalyst layer models will be put to use to unravel correlated changes in physical properties and performance that have been widely observed when the Pt loading of catalyst layers was drastically reduced [7,8]. {Reference on back of flyer}

Tuesday, February 12th

1:00 – 1:50PM | Spahr Auditorium

References

[1] J. Huang, A. Malek, J. Zhang and M.H. Eikerling, Unifying theoretical framework for deciphering the oxygen reduction reaction on platinum, Phys. Chem. Chem. Phys., in press.
[2] J. Huang, A. Malek, J. Zhang and M.H. Eikerling, Non-monotonic Surface Charging Behavior of Platinum: A Paradigm Change, J. Phys. Chem. C 120, 13587-13595 (2016).
[3] J. Huang, T. Zhou, J. Zhang, M. Eikerling, Double Layer of Platinum Electrodes: Non-Monotonic Surface Charging Phenomena and Negative Double Layer Capacitance, J. Chem. Phys. 148, 044704 (2018).
[4] K. Malek, T. Mashio, and M. Eikerling, Microstructure of Catalyst Layers in Polymer Electrolyte Fuel Cells Redefined: A Computational Approach, Electrocatalysis 2, 141-157 (2011).
[5] A. Nouri-Khorasani, K. Malek, A. Malek, T. Mashio, D.P. Wilkinson, M.H. Eikerling, Molecular modeling of the proton density distribution in a water-filled slab-like nanopore bounded by Pt oxide and ionomer, Catalysis Today 262, 133-140 (2016).
[6] T. Muzzaffar, T. Kadyk, and M. Eikerling, Physical Modeling of the Proton Density Distribution in Active Nanopores of the Cathode Catalyst Layer in PEM Fuel Cells, Electrochim. Acta 245, 1048-1058 (2017).
[7] Polymer Electrolyte Fuel Cells – Physical Principles of Materials and Operation, M. Eikerling and A.A. Kulikovsky, CRC Press, Boca Raton, 2014.
[8] T. Muzaffar, T. Kadyk, and M. Eikerling, Tipping Water Balance in Polymer Electrolyte Fuel Cells with Ultra-Low Pt Loading, Sust. Energy Fuels 2, 1189-1196 (2018).