

# Symposium

## Electrochemical Engineering for the 21<sup>st</sup> Century

in honor of Prof. Richard C. Alkire

217<sup>th</sup> ECS Meeting, Vancouver, Canada

### Symposium is open for abstract submission

Future trends in electrochemical engineering will be influenced by the need to control processes at the molecular scale. This symposium focuses on the role of molecularly coupled electrochemical engineering in addressing future technology challenges of the 21<sup>st</sup> Century. It features two prominent keynote speakers in each of three topic areas. Papers are solicited in all three areas.



Tetsuya Osaka



Dieter Kolb

**Session 1:** Experimental and theoretical methods for understanding and describing behavior in electrochemical systems at the molecular level.



Richard Alkire



Linda Petzold

**Session 2:** Engineering methods and simulation algorithms that enable coupling to molecular scale processes for the design, control and optimization of entire, realistic systems.



Mark Verbrugge



Lubomyr Romankiw

**Session 3:** Use of molecular understanding, design and/or control to address 21<sup>st</sup> Century electrochemical engineering applications.

Questions and inquiries  
should be sent to the  
symposium organizers:

- John Harb, Brigham Young University, e-mail: john\_harb@byu.edu
- Lili Deligianni, IBM Research, e-mail: lili@us.ibm.com
- Kurt Hebert, Iowa State University, e-mail: krhebert@iastate.edu
- James Fenton, University of Central Florida, e-mail: jfenton@fsec.ucf.edu
- Richard Varjian, AIC Labs, e-mail: richard.varjian@apicap.com
- Venkat Subramanian, Tennessee Tech University, email: VSubramanian@tntech.edu

## Establishment of Electrochemical Device Engineering

Tetsuya Osaka

Faculty of Science and Engineering, Waseda University  
3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555 Japan

Electrochemical nanotechnology has produced a variety of materials with the nanometer scale. These nano-scale materials have made it possible to miniaturize electric devices, and they are fascinating because of their characteristics, which are remarkably different from bulk materials [1]. I have been serving as advisory board of the series of symposia entitled "International Symposium on Electrochemical Micro- and Nanosystem Technologies (EMNT)," which started in 1996 and was held every two years. From the initial proposal to launch the EMNT symposia during the ECS Fall Meeting in 1994, we were convinced that the concept of EMNT should play an important role in leading electrochemical science and engineering to a successful future.

In the past few decades, our group has been conducting our research based on the philosophy of "creating new designs for the interface between the electrode and electrolyte at an atomic or molecular level," particularly in view of the application of electrochemical nanotechnology to the developments of advanced materials and devices [2], e.g., magnetic recording materials, interconnects in ULSI devices, energy devices such as Li batteries and micro-sized fuel cells, and chemical/bio-sensors.

### Electrochemical Device Engineering

Our research project entitled "Establishment of Electrochemical Device Engineering," under the Grant-in-Aid for Specially Promoted Research from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan, started in 2008. The object of this project is to establish the basic concept for device fabrication process on the basis of the results of our study on the practical application of electrochemical nanotechnology.

This 5-year project is particularly focused on the development of energy devices and sensor devices with three- or two-dimensional designs of interface. As for the energy devices, the design and control of three-dimensional microstructure and interface for the electrode and electrolyte materials are intensively investigated for developing high-performance Li secondary batteries and on-chip fuel cells. The sensor devices are investigated mainly from the viewpoint of two-dimensional design of the interface. In addition, nanoparticles of functional materials [3] are investigated as a zero-dimensional system, of which two- or three-dimensional assemblies are also important subject of this project. Figure 1 shows the concept of project.

### Development of Chemical/Bio-sensors

The study on the sensor devices is being focused on two-dimensional design and control of interface at the molecular level, considering the fact that not only small molecules or ions but also proteins or DNA can be the target of chemical/bio-sensing.

Following the successful development of organosilane monolayer-modified SiO<sub>2</sub>-gate field effect transistors (FETs) with a high degree of chemical durability [4], we have been researching FET-type chemical/bio-sensors with high degrees of sensitivity and good stability in aqueous solutions, based on the

molecular-level design of the gate/solution interface for both *recognition/detection* and *reference* FETs. In regard to the *reference* FET, the nano-scale surface morphology of the octadecylsilane (ODS) monolayer-modified SiO<sub>2</sub> gate, which is originated from ODS coagulation, was found to affect pH and ionic responses of the FETs [5]. Regarding the antibody-immobilized gate FET, as an example of *recognition/detection* FETs, the voltage-sweep treatment of glutaraldehyde-modified SiO<sub>2</sub> gate prior to the immobilization of antibody was found to improve the orientation and two-dimensional packing of antibody molecules immobilized on the gate, leading to high degrees of reproducibility and stability [6].

In our research on monolayer-modified electrodes, the Au electrode modified with monolayer of homocysteine (Hcy) was demonstrated to achieve high-accuracy recognition of mirror-image isomers, or enantiomers, of chiral molecules based on the formation of Cu complex at the electrode/electrolyte interface, in which Hcy in monolayer and target molecules coordinate to Cu(II) [7]. For the further expansion of this result, the development of Au-coated SiO<sub>2</sub>-gate FET and its application to chiral sensors, which can detect the charge due to the Cu complex formation on the monolayer-modified Au, are in progress.

Three-, two-, and zero-dimensional designs for the electrode/electrolyte interface based on electrochemical nanotechnology are believed to contribute to the establishment of "Electrochemical Device Engineering."

### References

- [1] T. Osaka, "New Developments in Electrochemical Nanotechnology", Plenary Lecture at PRiME 2008, October 13, 2008 in Honolulu, Hawaii.
- [2] T. Osaka, *Chem. Record*, **4**, 346-362 (2004).
- [3] T. Osaka, H. Iida, S. Tominaka, T. Hachisu, *Israel J. Chem.*, **48**, 333-347 (2008).
- [4] D. Niwa, T. Homma, T. Osaka, *Jpn. J. Appl. Phys.*, **43**, L105-L107 (2004).
- [5] S. Kuroiwa, J. Wang, D. Satake, S. Nomura, T. Osaka, *J. Electrochem. Soc.*, **156**, J67-J74 (2009).
- [6] S. Hideshima, T. Nakanishi, T. Osaka, 216<sup>th</sup> ECS Meeting, Abs# 1628, October 5, 2009 in Vienna, Austria.
- [7] M. Matsunaga, T. Nakanishi, T. Asahi, T. Osaka, *Electrochem. Commun.*, **9**, 725-728 (2007).

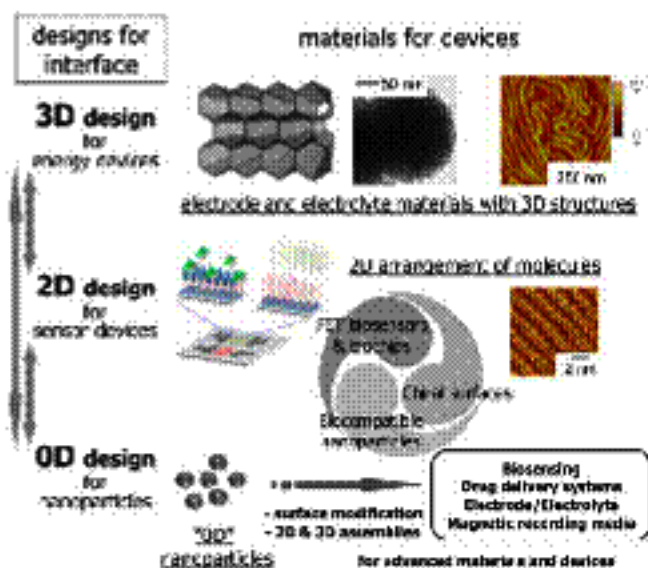


Figure 1. Concept of the project "Establishment of Electrochemical Device Engineering."

# 217th ECS Meeting - Vancouver, Canada

April 25 - April 30, 2010

## PROGRAM INFORMATION

### F2 - Electrochemical Engineering for the 21st Century (dedicated to Richard C. Alkire)

Electrodeposition/Industrial Electrochemistry and Electrochemical  
Engineering/Corrosion/Energy Technology

Monday, April 26, 2010

Georgia B, 2nd Floor, Hyatt

Multiscale Modeling

Co-Chairs: Venkat Subramanian and Linda Petzold

Time	Abs#	Title and Authors
08:00	1240	<a href="#">Water Transport in the Ionomer-Phase and Across Its Interfaces in Catalyst Coated Membranes for Proton Exchange Membrane Fuel Cells</a> V. Gurau and J. Mann (Case Western Reserve University)
08:20	1241	<a href="#">Surface Morphology of Lithium Metal Anodes</a> M. Karulkar and J. Adams (Ford Motor Company)
08:40	1242	<a href="#">Continuum and Multiscale Modeling of Performance Curves and Capacity Fade in Lithium-Ion Batteries</a> V. Subramanian, V. Ramadesigan, R. N. Methekar (Washington University), K. Chen and R. Braatz (University of Illinois at Urbana-Champaign)
09:00	1243	<a href="#">Formation of Localized Corrosion-Relevant Surface Defects on Aluminum: Experimental Studies and Kinetic Monte Carlo Simulation</a> K. Hebert, G. Zhang, J. Ai (Iowa State University) and G. Stafford (National Institute of Standards and Technology)
09:20	1244	<a href="#">Simulation of Three-Dimensional Solid-by-Solid Model and Application to Electrochemical Engineering</a> Y. Kaneko (Kyoto University), Y. Hiwatari (Toyota Physical and Chemical Research Institute), K. Ohara and F. Asa (C. Uyemura & Co., Ltd.)
09:40		Intermission (20 Minutes)
10:00	1245	<a href="#">(Keynote) Electrochemical Engineering: The Need for Next-Generation Methods</a> R. Alkire (University of Illinois)
10:40	1246	<a href="#">(Keynote) An Algorithm for Simulation of Electrochemical Systems with Surface-Bulk Coupling Strategies</a> M. Buoni (Los Alamos National Laboratory) and L. Petzold (University of California Santa Barbara)
11:20	1247	<a href="#">Characteristic Timescales in Multiscale Feature Metallization</a> J. D. Adolf and U. Landau (Case Western Reserve University)
11:40	1248	<a href="#">Adsorptive SPS Dissociation Within the c(2x2)-Cl Matrix on Cu(100) under Reactive Conditions: A Combined In Situ STM and DFT Study</a> N. T. Hai (University of Bern), W. Reckien (University of Bonn), A. Fluegel, M. Hahn, A. Wagner, D. Mayer (BASF SE), T. Bredow (University of Bonn) and P. Broekmann (University of Bern)

**Electrochemical Systems-Molecular/Nano**

Co-Chairs: John Harb and Daniel Schwartz

Time	Abs#	Title and Authors
------	------	-------------------

- 14:00 1249 [\(Keynote\) The Metallization of SAMs: Molecular Double Deckers](#) F. Eberle, M. Manolova, D. M. Kolb (University of Ulm), H. Boyen and M. Saitner (Hasselt University)
- 14:40 1250 [Metallization of DNA Origami Templates for the Fabrication of Nanoelectronic Circuits](#) J. Harb (Brigham Young University), J. Liu (Brigham Young University), Y. Geng, E. Pound, J. Ashton, S. Gyawali and A. Woolley (Brigham Young University)
- 15:00 1251 [Combined Electrochemical and In Situ STM Studies on the Redox-Activity of Leveler Additives](#) A. Fluegel (BASF SE), N. T. Hai (University of Bern), M. Hahn, A. Wagner, D. Mayer (BASF SE) and P. Broekmann (University of Bern)
- 15:20 1252 [Nanomanufacturing by Orchestrated Structure Evolution](#) S. Kitayaporn, S. Abbasi, K. Böhringer and D. Schwartz (University of Washington)
- 15:40 1253 [Nanosheet Formation by Electrodeposition and Its Application to Miniaturized Reference Electrodes](#) S. Safari-Mohsenabad (McMaster University), P. R. Selvaganapathy (McMaster University), A. Derardja (University of Batna) and M. J. Deen (McMaster University)
- 16:00 1254 [Creating Metallic Conductivity in TiO<sub>2</sub> Nanotubes](#) R. Hahn and P. Schmuki (University of Erlangen)
- 16:20 1255 [Density Functional Theory Study on the Oxidation Reactivity of Hypophosphite Ion as a Reductant for Electroless Deposition Process](#) M. Kunimoto, H. Nakai and T. Homma (Waseda University)

## Tuesday, April 27, 2010

Georgia B, 2nd Floor, Hyatt

### Electrochemical Systems-Fundamental

Co-Chairs: Kurt Hebert and Stanko Brankovic

- | Time  | Abs# | Title and Authors  |
|-------|------|--|
| 08:20 | 1256 | <a href="#">Wet Etching Process on Semiconductors: A Typical Electrochemical Engineering Challenge</a> A. Causier, M. Bouttemy, I. Gérard and A. Etcheberry (Institut Lavoisier UMR CNRS 8180)         |
| 08:40 | 1257 | <a href="#">Simulation of Cu Surface Morphology Evolution during Electropolishing</a> J. Thomas and S. R. Brankovic (University of Houston)  |
| 09:00 | 1258 | <a href="#">Porosity of Electrodeposited Cobalt Hard Gold: Effects of Reversed Pulse Current</a> Z. Liu (Columbia University), M. Zheng, R. Hilty (Tyco Electronics) and A. West (Columbia University) |
| 09:20 | 1259 | <a href="#">Direct Copper Plating on a RuTa Substrate</a> M. Nagar, A. Radisic (IMEC), K. Strubbe (Ghent University) and P. Vereecken (IMEC)   |

### Electrochemical Devices

Co-Chairs: Lili Deligianni and James Fenton

- | Time    | Abs# | Title and Authors   |
|---------|------|---|
| → 10:00 | 1260 | <a href="#">(Keynote) Establishment of Electrochemical Device Engineering</a> T. Osaka (Waseda University)  |
| 10:40   | 1261 | <a href="#">One-Dimensional Molecular-Junction Arrays Fabricated Using Anodic Aluminum Oxide Templates</a> Y. Song, J. Fang and Z. D. Chen (University of Kentucky)   |
| 11:00   | 1262 | <a href="#">Future Challenges in Electrochemical Engineering from Microelectronics to Solar Thin Films</a> H. Deligianni (BM T.J. Watson Research Center), Q. Huang (IBM T.J. Watson Research Center), L. T. Romankiw (BM T.J. Watson Research Center), R. Vaidyanathan, S. Ahmed (IBM T.J. Watson Research Center), S. Jaime, P. Grand, V. Charrier and O. Kerrec (Nexcis Photovoltaic Technology) |
| 11:20   | 1263 | <a href="#">Analysis and Control of Plating Baths in the Electrodeposition of Copper Indium</a>   |