

# Japanese Swiss Energy Materials Workshop

March 7-9, 2016

Empa Akademie  
Dübendorf, Switzerland



Schweizerische Eidgenossenschaft  
Confédération suisse  
Confederazione Svizzera  
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Swiss Confederation

Federal Department of Economic Affairs,  
Education and Research EAER  
State Secretariat for Education,  
Research and Innovation SERI



Empa

Materials Science and Technology

ETH zürich



科学技術振興機構  
Japan Science and Technology Agency



Front picture: False-colored scanning electron microscopy image of a recrystallized ceria fiber used for CO<sub>2</sub> reduction cycles

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# **Japanese Swiss Energy Materials Workshop**

**March 7 – 9, 2016**

**Empa Akademie**

**Dübendorf, Switzerland**

**Programme and Abstracts**

## Background

The Japan Science and Technology Agency (JST), ETH Zurich in its function as Swiss Leading House and Empa are jointly organizing the Japanese Swiss Energy Materials Workshop on March 7-9, 2016. The workshop is part of the bilateral Japanese-Swiss Science and Technology Programme established in 2008 with the aim of fostering scientific relations between the two countries, and follows in a series of similar events held in 2008, 2009, 2013 and 2015 respectively. The Energy Materials workshop will connect top scientists working on energy conversion and storage materials from leading Japanese and Swiss institutions and promote exchange and cooperation between researchers by presenting the frontiers of energy materials research in the two countries. It aims at connecting in particular young scientists and complements the available instruments for funding joint research projects and the exchange of scientists available between Japan and Switzerland.

## Concept

The workshop-format as opposed to a conference was intentionally chosen to encourage maximum interaction between the participants. All participants are thus invited to also bring a poster to illustrate their research and ample space for discussion and networking will be provided. Posters will be on display all day and in addition to the dedicated poster sessions coffee breaks and lunches can be used to discuss posters. Please do also observe that the 20 minutes slots for speakers include 17 minutes of presentation and 3 minutes of questions. Short questions from all the audience directly to individual speakers are allowed and encouraged any time during the workshop.

## Schedule

Monday, March 7	Workshop Opening, Scientific Sessions, Conference Dinner
Tuesday, March 8	Scientific Sessions, Conclusions, Zurich City Tour
Wednesday, March 9	Laboratory Tour Empa

## Organization

The workshop is organized by Dr. Corsin Battaglia, Empa and Prof. Motoko Kotani, Tohoku University as scientific chairs. JST and ETH Zurich in its role as Swiss Leading House of the Japanese-Swiss Science and Technology Programme are in charge of the administrative organization and provide funding of the workshop through the bilateral programme supported by the Swiss State Secretariat for Education, Research and Innovation (SERI).

## Scope of the Workshop

The year 2014 marked an important anniversary in the bilateral relations between Switzerland and Japan, established 150 years ago with the signing of the first trade and friendship agreement. The high level of excellent collaborative research, especially in the field of energy technologies, is proof for the close relationship between the two countries. Indeed, a fruitful event entitled the “Energy Technology Research Workshop” was held in Gstaad-Saanen in the Swiss Alps from 9-12 March 2014, and more than 60 people, including world-leading researchers in the field, attended to openly exchange their active opinions.

The deployment of sustainable energy technologies is of great importance for both countries which share several common features; a rugged, mountainous territory of which only a small part may be used for agriculture, and few natural resources. To accelerate the large scale deployment of these technologies, it is essential to enable scientific breakthroughs through the discovery of novel high performance **energy materials** for photovoltaics, batteries, fuel cells and electrolysis/photocatalysis, employing new approaches for materials design including mathematics and information science. To strengthen collaborative research between young researchers in Japan and Switzerland and promote future joint bilateral research projects, the workshop brings together 28 outstanding Japanese and Swiss researchers that will present their frontier research on energy materials. We hope that this workshop contributes to discover synergies that enable Japan and Switzerland to move towards a sustainable energy society.

Scientific Workshop Co-Chairs

Motoko Kotani, Advanced Institute for Materials Research, Tohoku University

Corsin Battaglia, Empa, Swiss Federal Laboratories for Materials Science and Technology

# Workshop Programme

## Monday 7 March 2015

08:30-09:00 **Opening Official Talks** (Chair: [Corsin Battaglia](#), Scientific Chair, Empa)

[Brigitte Buchmann](#) (Member of Board of Directors, Head of Department Mobility, Energy and Environment, Empa)

[Sotaro Ito](#) (Deputy Executive Director, JST)

[Matthias Frey](#) (Head Science and Technology Office, Swiss Embassy Tokyo)

09:00-09:10 **Goals of the Workshop**

[Motoko Kotani](#) (Scientific Chair, Tohoku University)

09:10-10:50 **Scientific Session 1: Photovoltaics** (Chair: [Corsin Battaglia](#))

[Kenjiro Miyano](#) (NIMS)

“Lead Halide Perovskite Photovoltaic as a Model  $p-i-n$  Diode”

[Monica Morales-Masis](#) (EPFL)

“High Performance Transparent Conductive Oxides: from Fundamentals to Applications”

[Takashi Koida](#) (AIST)

“Transparent conductive and semi-conductive oxides for photovoltaics”

[Stephan Bücheler](#) (Empa)

“Thin film solar cells with efficiencies above 20%”

[Qing Shen](#) (The University of Electro-Communications)

“Quantum Dot and Perovskite Solar Cells: Interface Engineering, Photoexcited Carrier Dynamics and Mechanism for Improving Photovoltaic Performance”

10:50-11:10 **Coffee Break**

11:10-12:10 **Scientific Session 2: Emerging Concepts** (Chair: [Motoko Kotani](#))

[Eiji Saitoh](#) (Tohoku University)

“Spin current generators”

[Oleg Yazyev](#) (EPFL)

“Computational search for novel topological materials”

[Tsuneya Yoshida](#) (RIKEN)

“Correlation effects on topological insulators in one dimension”

12:10-13:30 **Lunch Break**

13:30-14:30 **Scientific Session 3: Batteries A** (Chair: [Corsin Battaglia](#))

[Shinichi Orimo](#) (Tohoku University)

“Complex Hydrides for Energy Device Research”

[Maksym Kovalenko](#) (ETH Zurich/Empa)

“Nanoscale anode and cathode materials for (Li/Na/Mg/Al)-ion batteries”

[Taro Hitosugi](#) (Tokyo Institute of Technology)

“Intrinsic interface resistance across LiPON/LiCoO<sub>2</sub> interfaces”

14:30-16:00 **Poster Session with Coffee**

16:00-17:00 **Scientific Session 4: Photocatalysis/Electrolysis/Catalysis A** (Chair: Corsin Battaglia)

[Ulrich Aschauer](#) (University of Bern)

“Functional defects in oxides“

[Peter Broekmann](#) (University of Bern)

“Power to Value: Electrochemical Conversion of CO<sub>2</sub>“

[Peka Peljo](#) (EPFL)

“Heat-to-Power Conversion and Hydrogen Production with Redox Flow Batteries”

**Transfer**

18:00-21:00 **Conference Banquet**

Restaurant Saal, Dübendorf

Hosted by [Gian-Luca Bona](#), Empa Director

## Tuesday, 8 March 2015

08:50-10:30 **Scientific Session 5: Batteries B** (Chair: [Corsin Battaglia](#))

[Itaru Honma](#) (Tohoku University)

"Supercritical fluid processing of nanocrystals, nanosheets, thin films for Li-ion batteries, Solar cells and Graphenes"

[Claire Villevieille](#) (Paul Scherrer Institute)

"Operando techniques to probe battery materials"

[Yoshitaka Tateyama](#) (NIMS)

"DFT samplings reveal atomistic mechanisms around electrolyte-electrode interfaces in batteries"

[Corsin Battaglia](#) (Empa)

"A new class of solid-state electrolytes for lithium ion batteries with conductivities near liquid electrolytes"

[Michihisa Koyama](#) (Kyushu University)

"Multi-Physics Simulation of Porous Electrode for Lithium Ion Battery"

10:30-10:50 **Coffee Break**

10:50-12:10 **Scientific Session 6: Data Driven Design** (Chair: [Motoko Kotani](#))

[Koji Tsuda](#) (The University of Tokyo)

"Machine Learning for Materials Discovery: Virtual Screening and Bayesian Optimization"

[Akihide Kuwabara](#) (Japan Fine Ceramics Center)

"First Principles Calculations of Diffusion and Defect Formation Mechanism in Solid State Ionic Conductors"

[Teodoro Laino](#) (IBM RSM Zurich Laboratory)

"Cognitive design of novel solid state electrolytes"

[Motoko Kotani](#) (Tohoku University)

"Mathematical Challenge to a New Phase of Materials Science"

12:10-13:30 **Lunch Break**

13:30-14:30 **Scientific Session 7: Photocatalysis/Electrolysis/Catalysis B** (Chair: [Corsin Battaglia](#))

[Kenji Miyatake](#) (University of Yamanashi)

"Molecular design, synthesis, and properties of anion exchange membranes for alkaline fuel cells"

[Raffaella Buonsanti](#) (EPFL)

"Colloidal Chemistry to advance solar-to-fuel conversion studies"

[Shintaro Ida](#) (Kyushu University)

"Nanosheet photocatalysts for water splitting"

14:30-16:00 **Poster Session with Coffee**



16:00-17:00 **Scientific Session 7 continued**

[Markus Niederberger](#) (ETHZ)

"Nanoparticles as Building Blocks for 2- and 3-Dimensionally Structured Materials for Energy Applications"

[Stephen Lyth](#) (Kyushu University)

"Heteroatom-doped Carbons for Electrochemical Energy Conversion"

[Matthias Koebel](#) (Empa)

"Custom-tailored Carbon Materials for Energy Upgrading & Conversion"

17:00-17:15 **Final Discussion and Conclusions**

[Scientific Chairs](#)

18:30-19:30 **Guided Zurich City Tour**

19:30-21:00 **Casual Dinner at Restaurant Zunfthaus, Zurich**

E.g. Zeughauskeller tbc

## Wednesday 9 March 2015

08:30-11:00 **Lab Tour at Empa**

In up to 5 groups for 5x30 min

11:00-11:30 **Farewell**



**Abstracts and CVs for Scientific  
Sessions  
(speakers according to programme)**



**Monday March 7**  
**Session 1**  
**Photovoltaics**



## Kenjiro Miyano

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### Previous Positions

1991-2012 professor, University of Tokyo

1988-1991 associate professor, University of Tokyo

1983-1988 associate professor, Tohoku University

### Research Interests

Condensed matter physics, optical properties of solids (nonlinear optics, pump-probe spectroscopy, photoinduced phase transitions, plasmonics)

### Lead Halide Perovskite Photovoltaic as a Model *p-i-n* Diode

Kenjiro Miyano, Neeti Tripathi, Masatoshi Yanagida, and Yasuhiro Shirai  
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**Keywords:** *perovskite photovoltaics, electronic characterization, intrinsic semiconductor*

The energy conversion efficiency of photovoltaics (PVs) based on lead halide perovskite has demonstrated the fastest improvement in the photovoltaic history in the past few years. It is most amazing that above 20% efficiency has been attained with facile spin-coating technology. Although it has been suggested from the early stage of the current surge of research that the electronic working of these PVs is a simple *p-i-n* diode, the evidences are piecewise and no coherent study has been done. Here, we present results of a set of experiments that are compelling enough for us to conclude that perovskite PVs are close cousins of inorganic thin film solar cells. Many research tools develop in the latter field are readily available: in fact they should be fully exploited by those engaged in perovskite PV research.

The utmost important factor for a comprehensive study is to have samples with stable and reproducible electronic characteristics; an obvious requirement but many published data are plagued by the irreproducibility generically termed as hysteresis. With hysteresis-free samples, however, very simple picture emerges. 1) the current/voltage relationship is well described by the textbook semiconductor equation, 2) the AC characteristics are mostly governed by the intrinsic perovskite layer with modification by the photo-activated defect as is typical for thin film PVs, 3) the Mott-Schottky plot of the capacitance is in perfect accord with the presence of thick intrinsic perovskite layer between the *p*- and *n*- contacts. The perovskite layer acts as an ideal intrinsic layer. The outstanding question is why it is so, despite the numerous defects and impurities.

References : Miyano et al., Appl. Phys. Lett. **106**, 093903 (2015), Acc. Chem. Res. DOI: 10.1021/acs.accounts.5b00436, Tripathi et al., J. Mater. Chem. A, **3**, 12081 (2015), ACS

Appl. Mater. Interfaces DOI: 10.1021/acsami.5b11286 (2016)



## Monica Morales-Masis

**Team leader of the Transparent Conductive Oxides (TCO) group.  
Ecole Polytechnique Fédérale de Lausanne (EPFL), Photovoltaics  
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### Previous Positions

- 2012 Postdoc at Leiden University, The Netherlands
- 2007-2011 PhD in Physics at Leiden University, The Netherlands.
- 2010 Visiting researcher (3 months) at National Institute for Materials Sciences (NIMS), Tsukuba-Ibaraki, Japan
- 2005-2007 M.Sc in Physics at Wright State University, Ohio, US
- 2000-2005 B.Sc in Physics at University of Costa Rica, Costa Rica.

### Research Interests

materials science, thin film technology, transparent conductive materials, photovoltaics, flexible and transparent electronics, OLEDs, optoelectronic devices, resistive switching materials, renewable energy technologies, sustainable development, technology transfer.

### High Performance Transparent Conductive Oxides: from Fundamentals to Applications

Monica Morales-Masis<sup>1</sup>, Quentin Jeangros<sup>1</sup>, Esteban Rucavado<sup>1</sup>, Federica Landuchi<sup>1</sup>, Lorenzo Fanni<sup>1</sup>, Ali Dabirian<sup>1</sup>, Stefaan de Wolf<sup>1</sup>, Aïcha Hessler-Wyser<sup>1</sup>, Christophe Ballif<sup>1</sup>

<sup>1</sup>Ecole Polytechnique Fédérale de Lausanne (EPFL), Institute of Microengineering (IMT), Photovoltaics and Thin-Film Electronics Laboratory, Rue de la Maladière 71b, 2002 Neuchâtel, Switzerland

**Keywords:** *transparent electrodes, solar cells, OLEDs, optoelectronic properties, microstructure*

Transparent conductive oxides (TCO) are widely used as electrodes in a range of novel optoelectronic technologies, such as high-efficiency solar cells and organic light-emitting diodes (OLEDs). Each application requires TCO electrodes with a specific set of properties, beyond those of wide-band optical transmittance and high conductivity. In this talk, we will present an overview of the activities at the Photovoltaics Laboratory of EPFL on the development of novel functionalized TCOs for solar cells and OLEDs. In order to improve device efficiencies (light emission in OLEDs, and light in-coupling in PV), we study the interrelation between film microstructure, carrier transport properties and their influence on the optoelectronic properties of the TCOs, as well as their thermal and environmental stability. Additionally, we work on replacing rare and critical elements from existing TCOs, in order to make the next generation of transparent electrodes economically viable and industrially robust. The combination of understanding the fundamental optoelectronic behaviour and the material properties, will in the future allow us to develop novel transparent electrodes by intelligent design.



## Takashi Koida

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### Previous Positions

2002-2004 Researcher, Nakamura Inhomogeneous Crystal Project, ERATO-JST

### Research Interests

- Oxide thin films, Thin film semiconductors, Solar cells

## Transparent conductive and semi-conductive oxides for photovoltaics

Takashi Koida

Research Center for Photovoltaics,

National Institute of Advanced Industrial Science and Technology (AIST)

**Keywords:** *Transparent conductive oxide, Oxide semiconductor, Photovoltaic cell, Heterojunction, Silicon, Chalcopyrite compound*

Transparent conductive oxides (TCOs) are wide band gap degenerated semiconductors popularly used in optoelectronic devices. TCO films are employed as transparent electrodes in solar cells, including Si heterojunction, Si thin-film, Cu(In,Ga)Se<sub>2</sub>, perovskite, and organic thin-film solar cells. The development of high-performance photovoltaic cells and modules has stimulated research on TCO films; namely, the improvement of the electrical and/or optical properties of existing TCO materials, the development of alternative TCO materials composed of naturally abundant and low-cost metals, and the development of new multifunctional TCOs and/or transparent semi-conductive oxides (TSOs) that can improve device performance. TCO and TSO materials are binary (In<sub>2</sub>O<sub>3</sub>, ZnO, SnO<sub>2</sub>, CdO, and Ga<sub>2</sub>O<sub>3</sub>) or multicomponent (In-Zn-O, Zn-Sn-O, and In-Ga-Zn-O). In this talk, I review our research on In<sub>2</sub>O<sub>3</sub>-based TCOs [1], focusing on high-mobility TCOs and their advantages in Si heterojunction [2] and Si thin-film solar cells [3]. In addition, I introduce our recent study on amorphous TSOs as electron transporting layers in solar cells, using a Cu(In,Ga)Se<sub>2</sub> thin-film solar cell [4].

[1]T. Koida, H. Fujiwara, M. Kondo, J. Non-Cryst Solids 354, 2805 (2008).

[2]T. Koida, H. Fujiwara, M. Kondo, Appl. Phys. Express, 1, 041501 (2008).

[3]H. Sai, T. Matsui, T. Koida, K. Matsubara, M. Kondo, S. Sugiyama, H. Katayama, Y. Takeuchi, I. Yoshida, Appl. Phys. Lett. 106, 213902 (2015).

[4]T. Koida, Y. Kamikawa-Shimizu, A. Yamada, H. Shibata, S. Niki, IEEE J. Photovolt. 5, 956 (2015).





## Stephan Buecheler

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### Research Interests

Single or multi-junction thin film solar cells based on  $\text{Cu}(\text{In,Ga})\text{Se}_2$  and  $\text{CdTe}$ , and perovskite semiconductors.

Metal oxide thin films as transparent conductive layers, surface passivation, diffusion barriers, or buffer layer for energy band alignment.

Solid state electrolytes and high potential cathodes for all-solid-state micro-batteries.

Applied research for industrial objectives in the field of solar energy.

Characterization methods of layers and interfaces, especially structural, chemical, optical and electrical properties.

### Thin film solar cells with efficiencies above 20%

S. Buecheler, B. Bissig, E. Avancini, R. Carron, T. Feurer, F. Fu, S. Pisoni, S. Nishiwaki, A.N. Tiwari

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**Keywords:** CIGS, Perovskite, Tandem, Solar Cells, Thin Film

Solar modules with power conversion efficiency beyond 20% produced by large area thin film deposition equipment will enable cost efficient solar electricity. The recent achievements on the development of low temperature processed  $\text{Cu}(\text{In,Ga})\text{Se}_2$  (CIGS) based solar cells with focus on the role of alkaline treatments will be discussed in this contribution. Further the combination of the CIGS cells with the hybrid organic-inorganic perovskite cells in tandem configuration will be presented.

Proper control of alkaline elements added to the CIGS absorber layer is a key aspect for the processing of high efficiency solar cells. Recently, we introduced a modified alkaline treatment of the absorber layer grown at low temperature, allowing the processing of flexible and lightweight devices with 20.4% efficiency.

The high efficiency of perovskite solar cells coupled with the large bandgap (tunable up to 2.3 eV) makes them ideal candidates as top cells in all-thin-film tandem devices with  $\text{Cu}(\text{In,Ga})\text{Se}_2$  (CIGS) as bottom cell. The development of NIR transparent top cell architectures is a prerequisite for successful development of highly efficient tandem devices. We report a hysteresis-free semi-transparent planar perovskite solar cell with remarkably high steady-state efficiency above 14%. In combination with low bandgap CIGS we demonstrate conversion efficiency above 20% in 4-terminal tandem configuration. Furthermore, the NIR transparent perovskite solar cells can be operated in bifacial mode resulting in substantial power enhancement.



## Qing Shen

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### Previous Positions

1995 Research Fellowship for Young Scientists (PD) of JSPS, The University of Tokyo  
 1995-1996 Research Assistant, The University of Tokyo  
 1996-2013 Assistant Professor, The University of Electro-Communications (UEC)  
 1998 Visiting Scientist of MIT and National Research Council of Canada  
 2009-2013 JST PRESTO Researcher  
 2013-present Associate Professor, The University of Electro-Communications (UEC)

### Research Interests

semiconductor nanomaterials and nanostructures, semiconductor quantum dot (QD) solar cells, photocatalysis, photoexcited carrier dynamics (injection, transfer, transport, charge separation and recombination) in various solar cells such as QD-based solar cells, perovskite solar cells, organic-inorganic hybrid solar cells and dye sensitized solar cells.

### **Quantum Dot and Perovskite Solar Cells: Interface Engineering, Photoexcited Carrier Dynamics and Mechanism for Improving Photovoltaic Performance**

Qing Shen,<sup>1</sup> Taro Toyoda,<sup>1</sup> and Shuzi Hayase<sup>2</sup>

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**Keywords:** *Quantum Dot, Perovskite, Solar Cell, Charge Separation, Recombination*

As one candidate of the next generation solar cells, colloidal quantum dot (CQD) based solar cells (CQDSCs) have attracted considerable interest and developed rapidly during the past few years. CQDSCs have some unique advantages such as the band-gap tunability, high absorption coefficient, multiple exciton generation (MEG) possibility and low cost for preparation. Although theoretical energy conversion efficiency of CQDSCs has been predicted to be about 44%, it is still less than 10% at present time. In this presentation, we would like to focus on how to improve the efficiencies of both QD sensitized solar cells and QD heterojunction solar cells by controlling the nano-interfaces and the mechanism for the improvement of the energy conversion efficiency of CQDSCs will be discussed.

On the other hand, the interest in organometal trihalide Pb perovskite (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>)-based solid-state hybrid solar cells has increased in recent years due to the high efficiencies achieved, with a record of over 20%, and the simple low temperature preparation method. Further improvements in the photovoltaic performance can be obtained by increasing the light harvesting in the NIR region up to 1000 nm. Recently, successful energy harvesting up to a wavelength of 1060 nm using Sn/Pb cocktail halide based perovskite materials has been achieved. In this presentation, we will also introduce our recent research results on the optical absorption properties, photoexcited charge separation and recombination dynamics at each interface in both Pb and Sn/Pb cocktail halide perovskites, and the relationships between these and the photovoltaic performance.

**Monday March 7**  
**Session 2**  
**Emerging Concepts**



## Eiji Saitoh

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### Previous Positions

2001-2006 Assistant Professor, Department of Physics, Keio University

### Research Interests

Physics of spintronics

### Spin current generators

Eiji Saitoh<sup>1-4</sup>

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<sup>2</sup>WPI-AIMR, Tohoku University, Japan

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**Keywords:** *spin current, spintronics, spin Hall effect, spin Seebeck effects*

I will give an introduction to the concept and various fascinating phenomena of spin-current science. Generation and utilization of spin current, a flow of spin angular momentum of electrons in condensed matter, are the key challenge of today's nano magnetism and spintronics. The discovery of the inverse spin Hall effect has allowed researchers to detect and utilize spin current directly, and, since then, many spin-current driven effects have been discovered, including spin Seebeck effects, light-spin conversion, sound-spin conversion, and motion-spin conversion. Spin Seebeck effects refer to spin-current generation from a temperature gradient, where spin's non reciprocity allows it to rectify thermal fluctuation into unidirectional spin current; spins, working as a natural rectifier in magnets, may thus provide a versatile mechanism of energy conversion in condensed matter. Spin micro mechanics, one of more recent topics, will also be covered.



## Oleg Yazyev

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### Previous Positions

2009-2011 Postdoc, University of California, Berkeley

2003-2009 PhD and postdoc, EPFL

### Research Interests

graphene, 2D materials, topological insulators, defects, electronic transport, magnetism, first-principles calculations, materials discovery

## Computational search for novel topological materials

Oleg V. Yazyev<sup>1</sup>

<sup>1</sup> Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

**Keywords:** *topological insulators, first-principles calculations*

A large number of different topological electronic phases that can be realized in materials have been predicted recently. While many strong  $Z_2$  topological insulators have been found within the family of layered bismuth and antimony chalcogenides, solid experimental confirmations of materials realizing other topological phases, such as the weak  $Z_2$  topological insulators, topological crystalline insulators, Dirac and Weyl semimetals, are still very scarce. We have developed a methodology for identifying materials hosting various topological phases among known compounds. Our approach is based on the automated high-throughput screening of online databases of experimental crystallographic structures. Initial sampling is performed using simple criteria such as the size of band gap, the strength of spin-orbit coupling and crystallographic space group. The topological invariants of materials within the sample are computed from first principles using the z2pack approach [1,2]. One successful prediction followed by the experimental confirmation will be discussed in detail [3]. A new  $Z_2$  topological insulator was discovered in quasi-one-dimensional  $\beta$ -Bi<sub>4</sub>I<sub>4</sub>. The electronic structure of  $\beta$ -Bi<sub>4</sub>I<sub>4</sub>, characterized by  $Z_2$  invariants (1;110), is in proximity of both the weak TI phase (0;001) and the trivial insulator phase (0;000). Our angle-resolved photoemission spectroscopy measurements on the (001) surface reveal the presence of highly anisotropic Dirac fermions.

[1] A. A. Soluyanov and D. Vanderbilt, Phys. Rev. B **83**, 235401 (2011)

[2] D. Gresch, A. A. Soluyanov, D. Vanderbilt, G. Autès, O. V. Yazyev, D. Ceresoli, and M. Troyer, *in preparation*

[3] G. Autès et al., Nature Materials **15**, 154 (2016).



## Tsuneya Yoshida

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### Previous Positions

2011-2014 Kyoto University

### Research Interests

- Condensed matter physics, strongly correlated electron systems

### Correlation effects on topological insulators in one dimension

T. Yoshida<sup>1</sup>, R. Peters<sup>2</sup>, S. Fujimoto<sup>3</sup>, and N. Kawakami<sup>2</sup>

<sup>1</sup>RIKEN

<sup>2</sup>Division of Physics, Kyoto University

<sup>3</sup>Department of Materials Engineering Science, Osaka University

**Keywords:** *topological insulators, strongly correlated systems*

Topological band insulators show various interesting phenomena due to symmetry protected gapless excitations at the boundary. Recently, realization of this phase is proposed for  $d$ - ( $f$ -) electron systems. In these systems, correlation effects and topological properties are expected to trigger off exotic behaviors; for instance, a topological Mott insulator where edge modes in the single-particle excitations are gapped while those in the spin excitations remain gapless due to topological properties in bulk[1]. However, this exotic phase is proposed only by a simple mean-field theory and establishment of this phase by solid approaches is still lacking.

In order to study topological Mott insulators, we analyze a correlated topological insulator in one dimension[4,5]. Our analysis based on density-matrix renormalization group shows clear evidence of this phase and reveals that relations between symmetries and edge modes in the single-particle spectrum. Furthermore, we also analyze properties of the topological phase transition induced by correlation effects and elucidate intriguing behavior of an unconventional topological phase transition accompanied by zeros of the Green's function instead of gap-closing in the single-particle spectrum [5].

[1] D. A. Pesin, and L. Balents, Nat. Phys. **6** 376-381 (2009).

[2] H. Li and F.D.M. Haldane, Phys. Rev. Lett. **101**, 010504(2008); F. Pollmann *et al.*, Phys. Rev. B **81**, 064439 (2010); A. M. Turner *et al.*, Phys. Rev. B **83**, 075102 (2011).

[3] V. Gurarie, Phys. Rev. B **83**, 085426 (2011).

[4] S.R. Manmana, *et al.*, Phys. Rev. B **86**, 205119 (2012).

[5] T. Yoshida *et al.*, Phys. Rev. Lett. **112**, 196404 (2014).



**Yuki Shiomi** (*Poster only*)

**Assistant Professor**  
**Institute for Materials Research, Tohoku University**

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**Previous Positions:**

2012-2013 assistant professor (Advanced Institute for Materials Research, Tohoku University), 2003-2012 students (University of Tokyo)

**Research Interests**

Spintronics, Topological materials, Condensed matter physics

**Spin-charge conversion induced by spin injection into topological insulators**

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**Keywords:** *spin injection, topological insulators, spin current*

Detection and manipulation of electrons' spins are key prerequisites for spin-based electronics or spintronics. In this presentation, I will report successful spin injection into the surface states of topological insulators by using a spin pumping technique. By measuring the voltage that shows up across the samples as a result of spin pumping, we demonstrate that a spin-electricity conversion effect takes place in the surface states of bulk-insulating topological insulators  $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$  and Sn-doped  $\text{Bi}_2\text{Te}_2\text{Se}$ . In this process, the injected spins are converted into a charge current along the Hall direction due to the spin-momentum locking on the surface states. The present results reveal a great advantage of topological insulators as ideal spintronics devices for conversion between spin and electricity.

**References:** Y. Shiomi, K. Nomura, Y. Kajiwara, K. Eto, M. Novak, K. Segawa, Y. Ando, and E. Saitoh. "Spin-Electricity Conversion Induced by Spin Injection into Topological Insulators". *Phys. Rev. Lett.* 113, 196601 (2014). doi:<http://dx.doi.org/10.1103/PhysRevLett.113.196601>





**Monday March 7**  
**Session 3**  
**Batteries A**



## Shin-ichi ORIMO

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### Previous Positions

1993 - 1995: JSPS (Japan Society for the Promotion of Science) Research Fellow

1995 - 2002: Hiroshima University

(1998 - 1999: Max-Planck Institute for Metal Research, awarded by Humboldt and MEXT Fellowships)

2002 - Present: Tohoku University (PI, WPI-AIMR; Head of Section and Energy Mat. Center, IMR)

### Research Interests

Fundamentals and Energy-Related Applications of Hydrides

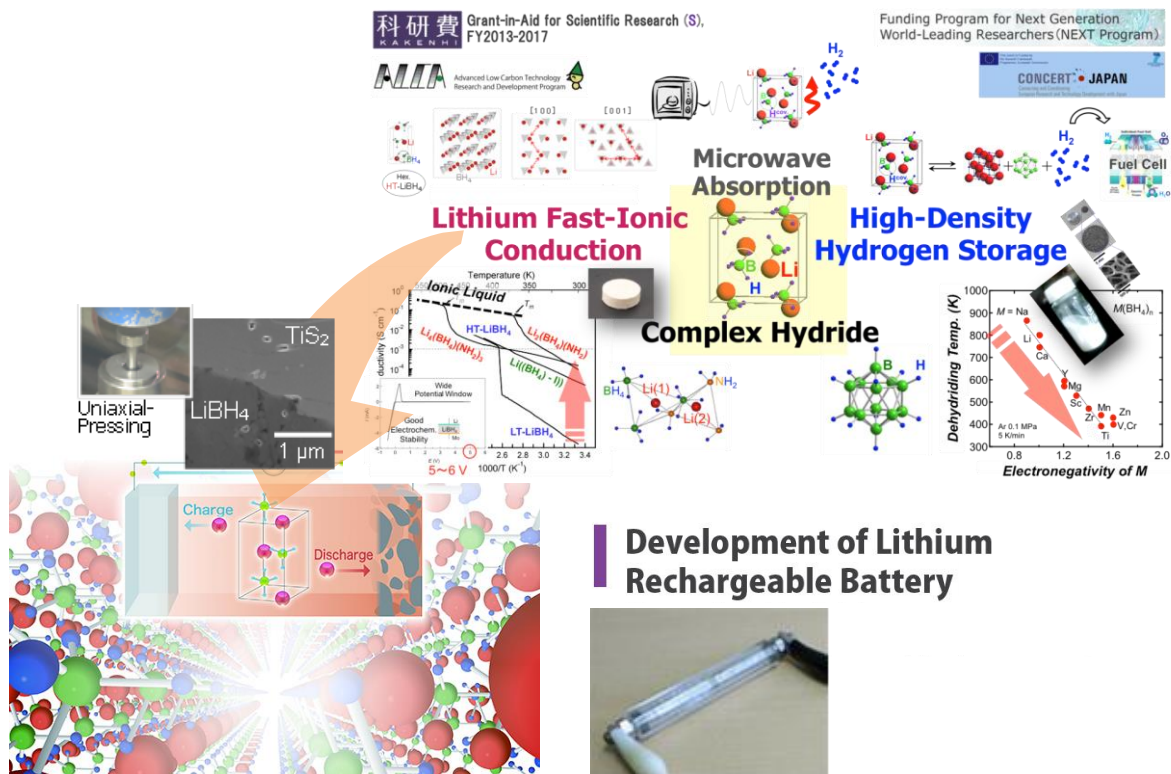
## Complex Hydrides for Energy Device Research

Shin-ichi ORIMO

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**Keywords:** High-Density Hydride, Superionic Conduction, Advanced Energy Device

Complex hydrides exhibit various energy-related functions as shown below; such as high-density hydrogen storage and microwave absorption for future fuel cell technologies [1], as well as lithium/sodium superionic conduction for energy devices [2-4]. In the presentation, intensive studies on fast-ionic conduction and development of lithium rechargeable battery using complex hydrides are to be explained.



- [1] S. Orimo et al., Chem. Rev. 107, 4111 (2007). (Research Front Paper, Times Cited: >1000)
- [2] M. Matsuo and S. Orimo, Adv. Energy Mater. (Review Article) 1, 161 (2011).
- [3] A. Unemoto et al., Adv. Functional Mater. (Feature Article) 103, 133903 (2014).
- [4] T.J. Udovic, S. Orimo et al., Chem. Comm. 50, 3750 (2014); Adv. Mater. 26, 7622 (2014).



## Maksym V. Kovalenko

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### Previous Positions

2008-2011 Postdoctoral Scholar, Department of Chemistry, University of Chicago, *with Prof. Dmitri V. Talapin*

2004-2007 Ph.D. study, Research Assistant, Institute of Solid State Physics, University of Linz, Austria, *with Prof. Wolfgang Heiss*

### Research Interests)

Chemistry, physics and applications of inorganic nanostructures; solid-state chemistry

- **Synthesis of semiconductor, metallic and magnetic nanocrystals:** size-, shape- and compositional control; nanocrystal heterostructures; self-assembly of nanocrystals into long-range ordered superlattices.
- **Nanocrystal surface chemistry:** all-inorganic surface capping ligands for integration of nanocrystals into electronic and optoelectronic devices.
- **Nanostructures for energy conversion and storage:** Novel nanostructured materials for Li-ion, Na-ion and Mg-ion batteries; molecular precursors and semiconductor nanostructures for solution-processable electronic, optoelectronic, thermoelectric, and photovoltaic devices.

### Nanoscale anode and cathode materials for (Li/Na/Mg/Al)-ion batteries

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ETH Zürich, Department of Chemistry and Applied Biosciences, CH-8093, Zurich,  
Switzerland  
and Empa-Swiss Federal Laboratories for Materials Science and Technology, CH-8600,  
Dübendorf, Switzerland

We will discuss the utility of monodisperse metallic nanocrystals as model anode material for Li-ion, Na-ion and Mg-ion batteries. Critical analysis of the advantages and shortcomings of nanostructured materials for practically usable batteries will be provided. Furthermore, novel strategies for designing low-cost magnesium-ion and aluminum-ion batteries using metallic magnesium and aluminum as anodes and carbonous materials as cathodes will be presented as well.



## Taro Hitosugi

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### Previous Positions

2007-2015 Associate Professor, Advanced Institute for Materials Research, Tohoku Univ.

### Research Interests

Solid-state chemistry/physics, solid-state electrochemistry, surfaces and interfaces

### Intrinsic interface resistance across LiPON/LiCoO<sub>2</sub> interfaces

Taro Hitosugi<sup>1,2</sup>

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<sup>2</sup> Department of Applied Chemistry, Tokyo Institute of Technology

**Keywords:** Solid-state lithium battery, Electrolyte/electrode interface, space-charge layer

We report the surprisingly low solid-electrolyte/electrode interface resistance of 8.6  $\Omega\text{cm}^2$  (Fig. 1), observed in  $\text{Li}_3\text{PO}_{4-x}\text{N}_x/\text{LiCoO}_2$  interfaces of thin-film lithium batteries.[1]

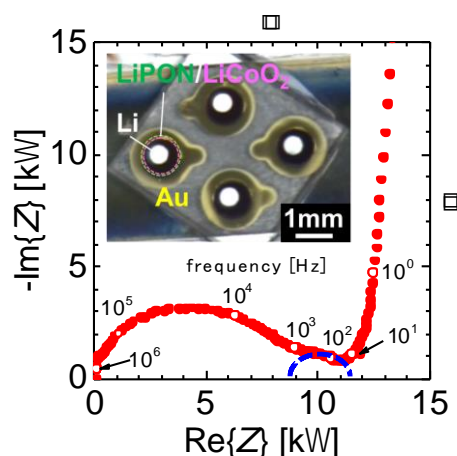
This value is an order of magnitude smaller than that presented in the previous reports on all-solid-state lithium batteries, and the value is also smaller than that observed in a liquid-electrolyte based lithium-ion batteries.

The observation of the low interface resistance indicates that intrinsic interface resistance across  $\text{Li}_3\text{PO}_{4-x}\text{N}_x/\text{LiCoO}_2$  is small, suggesting that the impact of negative space-charge layer effects at  $\text{Li}_3\text{PO}_{4-x}\text{N}_x/\text{LiCoO}_2$  interfaces is marginal.

Consequently, the results imply that it is possible to fabricate fast charging/discharging all-solid-state lithium batteries, which is superior to the existing liquid-electrolyte based Li-ion batteries

This work is supported by JST-CREST, JST-ALCA, and Kakenhi

[1] M. Haruta, S. Shiraki, T. Suzuki, A. Kumatani, T. Ohsawa, Y. Takagi, R. Shimizu, and T. Hitosugi, Nano Lett. 15, 1498 (2015).



**Fig. 1**

An impedance spectroscopy result obtained from a thin film all-solid-state lithium battery. The blue dashed curve indicates the contribution from a  $\text{Li}_3\text{PO}_{4-x}\text{N}_x/\text{LiCoO}_2$  interface. Note that we obtained very low interface resistance.

We speculate that the formation of a damage-less coherent interface led to the low-interface-resistance thin-film lithium batteries.

**Monday March 7**  
**Session 4**  
**Photocatalysis/Electrolysis/  
Catalysis A**



## Prof. Ulrich Aschauer

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### Previous Positions

2005-2008 PhD, Institute of Materials, EPFL, Switzerland

2008-2011 Postdoc, Department of Chemistry, Princeton University, USA

2011-2015 Postdoc, Materials Theory, ETH Zürich, Switzerland

### Research Interests

- Density functional theory calculations, mainly of oxides and oxynitrides
- Defect chemistry and interaction of defects with lattice, magnetic and electronic instabilities in complex oxides
- Functional properties resulting from defects in the bulk and at surfaces and interfaces
- Chemical reactions at surfaces, photocatalysis, water splitting

### Functional defects in oxides

Ulrich Aschauer<sup>1</sup>

<sup>1</sup> Department of Chemistry and Biochemistry, University of Bern, Switzerland

**Keywords:** *Density functional theory, Defects, Complex oxides, Photocatalysis*

Transition metal oxides are central for a wide range of applications. Intrinsic defects are ubiquitous in these materials and can have a marked effect on their properties. Control over the concentration and location of these defects could be used as a tuning knob for the resulting properties.

Based on the results of our density functional theory (DFT) calculations, I will discuss two routes to achieving such control over defect concentration and location: electric fields and epitaxial strain. In both cases our predictions are corroborated by experimental results from our collaborators, showing that external fields can indeed be used to achieve both instantaneous and permanent control over the defect population.

We will then look at prospects of such control: In the case of the complex oxide SrMnO<sub>3</sub> the interaction of defects with polar domain walls leads to the appearance of conductive nanodomains with potential applications for example in data storage. In the domain of photocatalysis I will show how the bulk/surface defect equilibrium can play a decisive role for the surface chemistry of TiO<sub>2</sub>.

As complex oxides and related anion substituted materials are being intensively researched for applications in solar energy conversion, affecting their surface chemistry via their defect population could prove crucial to achieve optimal performance of this novel class of materials.

## Peter Broekmann

Group leader and lecturer at the University of Bern

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### Previous Positions

2001-2006 Group leader at Bonn University (Bonn, Germany)

2006-2007 Senior Scientist at BASF SE (Electronic Materials, Ludwigshafen, Germany)

2007-present Group leader and lecturer at the University of Bern (Bern, Switzerland)

### Research Interests

Interconnect technology for advanced 3D packaging applications; Through-silicon-via (TSV) technology; additive-assisted plating processes; electrocatalysis; electrochemical CO<sub>2</sub> conversion (power to value approach); development of in operando methods

## Power to Value: Electrochemical Conversion of CO<sub>2</sub>

A. Dutta, M. Rahaman, V. KaliginediA. Kuzume, N.T.M. Hai, N. Luedi, T. Engel, M. Mohos and P. Broekmann

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**Keywords:** *Carbon dioxide, electroreduction, high surface area catalysts, metal foams, in operando analytical techniques*

A major challenge in the field of catalysis in general and electrocatalysis research in particular concerns the conversion of the green-house gas CO<sub>2</sub> into products of higher value. A promising approach makes use of excess of renewable electric energy (e.g. from solar or wind sources) to produce either fuels (e.g. methanol, methane) or other valuable stock chemicals (e.g. ethylene, formic acid, etc.) in terms of an electrocatalytic process. This approach is also known as *power to value* concept.

Whereas there are catalyst materials already available that significantly reduce the overpotential for CO<sub>2</sub> electroreduction there are still huge challenges left concerning the product selectivity of the CO<sub>2</sub> conversion and in particular the long term stability of the catalysts.

In this contribution we will discuss a new and versatile platform for the electrosynthesis of high surface area catalysts for the CO<sub>2</sub> conversion which is based on an additive assisted electrodeposition process of the catalyst material. It will be demonstrated that it is not only the specific chemical composition of the mesoporous alloy catalyst (e.g. Cu/Sn, Cu/Au or Sn/Ag alloys) which matters for the resulting product distribution but also the morphology of the mesoporous catalyst material (pore size, pore density etc.).

Our research is embedded into the CO<sub>2</sub> project of the **Swiss Competence Center of Energy Research (SCCER) Heat and Electricity Storage**. An interdisciplinary consortium of inorganic chemists (C. Coperet, ETHZ), organic chemists (P. Dyson, EPFL) and electrochemists (T.J. Schmidt, PSI, Villigen; P. Broekmann, University of Bern) develop new catalyst concepts for the CO<sub>2</sub> conversion for industrial applications.



## Pekka Peljo

**Team leader & Scientist, Laboratoire d'Electrochimie Physique et Analytique, École Polytechnique Fédérale de Lausanne**

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### Previous Positions

2010-2013 PhD student and Post-Doc, Aalto University, Finland

### Research Interests

- Energy conversion and storage, redox flow batteries, hydrogen,

### Heat-to-Power Conversion and Hydrogen Production with Redox Flow Batteries

Sunny Maye, Veronique Amstutz, Heron Vrubel, Hubert Girault, Pekka Peljo\*  
Laboratoire d'Electrochimie Physique et Analytique, École Polytechnique Fédérale de Lausanne, EPFL Valais, Sion, Switzerland

**Keywords:** waste heat, energy storage, flow batteries, hydrogen mobility

Currently the utilization of low temperature waste heat <200 °C is limited by the low efficiency for energy conversion and high system costs. We are working on a new approach based on thermo-electrochemical systems to convert low-grade heat first into a chemical energy that can then in turn be converted on demand into electricity through an electrochemical reaction. To illustrate this principle, a copper redox flow battery (RFB) based on complexation with acetonitrile was demonstrated [1]. The battery can be charged and discharged as a conventional battery, but it can also be charged by thermo-chemical reaction [1]. The thermal charging process, with the predicted maximum theoretical efficiency of the system is ca. 20%, can be integrated with any heat source of ca. 100 °C or more, including waste heat from industrial processes and power plants, but also geothermal sources and even heat from standard solar thermal collectors. Here, we will discuss the electrochemistry of copper in non-aqueous solvents, as well as the performance of the battery and the thermal regeneration.

Additionally, redox flow batteries (RFBs) can be used for indirect hydrogen evolution [2], or as a buffer for both renewable energy production and energy consumption by charging of electric cars. In the indirect hydrogen evolution the charged electrolytes of the vanadium RFB (VRFB) are chemically discharged in a separate catalytic bed of Mo<sub>2</sub>C catalyst to evolve hydrogen. This indirect approach was coupled with a commercial 10kW/40kWh VRFB and scaled up to kW scale [2].

We have also recently started a demonstration of a fueling station for both electric and fuel cell vehicles, based on 200kW/400kWh VRFB for DC-DC charge of electric vehicles and coupled with alkaline electrolyzer for hydrogen production for fuel cell cars.

[1] P. Peljo, *et al.*, Towards a thermally regenerative all-copper redox flow battery, *PCCP*. **16** (2014) 2831-2835.

[2] P. Peljo, *et al.*, All-Vanadium Dual Circuit Redox Flow Battery for Renewable Hydrogen Generation and Desulfurisation, *Green Chem.*, **in press**.



**Tuesday March 8**  
**Session 5**  
**Batteries B**



## Itaru Honma

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### Previous Positions

1985-1995 Lecturer, Dept.Chem.Eng.Univ.Tokyo, 1995-2010 Group Leader, AIST

### Research Interests

Renewable energy, Energy & Environmental Technology, Energy Conversion Devices

## Supercritical fluid processing of nanocrystals, nanosheets, thin films for Li-ion batteries, Solar cells and Graphenes

Itaru Honma

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Environmentally Friendly, low cost and large scale production processes of energy materials are quite important for the market penetration of renewable energy including solar cells, wind power as well as plug-in hybrid electric vehicles. For example, minimizing the cost of Lithium ion battery is crucial for accelerating of these green technologies. Lithium ion battery stores electrical energy in their electrode materials via Faradic reaction of the active materials under charge/discharge processes. The more number of electro/ions are involved in the electrode reaction, more energy density of the LIB cells are realized. The advanced materials processing employing supercritical fluid (SCF) has been applied to synthesize novel multi-electron redox compounds such as lithium metal phosphates, lithium metal silicates and lithium metal fluorophosphates, which are promising electrode materials with higher Li storage capacities. The supercritical fluid processes, a new kind of reaction media, offers versatile tools for morphology-controlled synthesis of nanocrystals owing to their unique properties such as gas like diffusivity, low viscosity and the density closer to that of liquid. The surface tension of SCFs completely vanishes above the critical point of the fluid which is of particular beneficial in controlling the surface and interface chemistry of the nano materials. Here, we report a rapid, one-pot SCF process for the preparation of size, and morphology control of  $\text{LiMPO}_4$ ,  $\text{Li}_2\text{MSiO}_4$  and  $\text{Li}_2\text{MPO}_4\text{F}$  (M: Fe, Mn, Co, Ni) nanocrystals [fig.1].

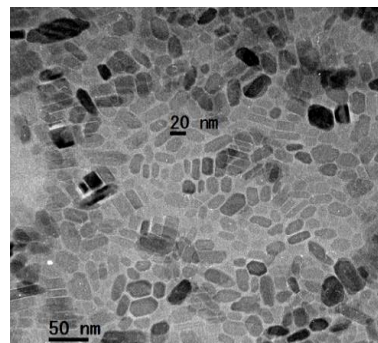


Fig.1 SCF fabrication of nanocrystals of  $\text{LiFePO}_4$

Additionally, wider applications of SCF processes are presented including the direct exfoliation synthesis of graphene nanosheet materials for secondary batteries & capacitor electrodes, transparent conducting electrodes. A low temperature ( $\sim 300^\circ\text{C}$ ) fabrication of solar cell compound semiconductor thin films such as  $\text{CuInSe}_2$  and  $\text{Cu}_2\text{ZnSnSe}_4$  in a 3D nanostructures. SCF process with catalytic reaction has been used to synthesize edge structure controlled nanographenes (fig.2), which are consisting of triangle shaped with Zig-Zag edge interfaces. The application of these nanographenes are promising for high energy density capacitor, magnetic fluids as well as secondary battery electrodes.

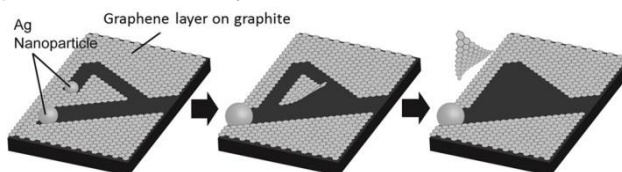


Fig.2 SCF fabrication of nanoGraphene



## Claire Villevieille

**Group Leader Battery Materials,  
Electrochemistry Laboratory  
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### Previous Positions & Research Interests

Claire Villevieille has been the leader of the Battery Materials group at the Paul Scherrer Institute in Switzerland since 2014. Her research is especially dedicated to study the reaction mechanisms of battery systems such as Li-ion, Na-ion, Li-S, and recently all-solid-state cells by means of various operando techniques. Moreover, her work centers on the proper design and/or adjustments of the measurement cells so that they meet the requirements of selected characterization techniques. Her research involves both, in-house devices as well as large facilities such as Swiss Light Source (PSI, Switzerland), Swiss Spallation Neutron Source (PSI, Switzerland), ERSF (Grenoble, France), ILL (Grenoble, France), and Soleil (Paris, France). In 2010 she accepted the position of a scientist at the Paul Scherrer Institute in Switzerland in the “Electrochemical Energy Storage Section” lead by Prof. Petr Novák. In 2006 she graduated with a Master degree in Materials Science (2006) at the University of Montpellier II in France. In 2009 she obtained her doctoral degree from the Science, Physics, and Chemistry Department (ICGM-AIME Laboratory) of the University of Montpellier II in France. Her doctoral studies focused on the conversion and insertion-based negative electrodes for Li-ion batteries and the elucidation of the complex reaction mechanisms using in situ X-Ray Diffraction (XRD), Mössbauer spectroscopy, SQUID measurements, etc. Her primary interests include solid state synthesis, electrochemical properties, and bulk–surface relationship of the various electrode materials.

### Operando techniques to probe battery materials

Claire Villevieille<sup>1</sup>

<sup>1</sup> Paul Scherrer Institute, Electrochemistry Laboratory, Villigen PSI, Switzerland

**Keywords:** *Batteries (Li-ion, Na-ion, Li-S), Operando techniques, bulk characterizations*

The Li-ion chemistry is the basis of the most advanced battery technology that offers the highest energy density, and therefore dominates the electronics field. However, its commercial success in the field of electric vehicles still requires further advances in performance, safety, and cost related issues. The same set of criteria concerns other systems based on alternative chemistries such as Na-ion and Li-S batteries. These novel systems utilizing less understood electroactive materials show new reaction mechanisms during electrochemical cycling, the understanding of which requires new characterization tools and techniques. Reliable, tailor-made electrochemical cells are employed to study the surface, the bulk, the interfaces, and finally to elucidate the reaction mechanisms. In this talk, different in situ/operando techniques, such as X-ray diffraction, neutron diffraction, X-ray absorption, and Raman spectroscopy used to characterize different systems such as Li-ion, Na-ion, and Li-S batteries will be presented.



## Yoshitaka Tateyama

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### Previous Positions

2007-2015 JST PRESTO researcher

2003-2004 University of Cambridge, visiting researcher

2001-2011 NIMS researcher/senior researcher/independent scientist

### Research Interests

computational materials science, DFT calculation studies on interfacial redox reactions, batteries, solar cells, (photo)catalysis

### DFT samplings reveal atomistic mechanisms around electrolyte-electrode interfaces in batteries

Yoshitaka Tateyama<sup>1,2,3</sup>

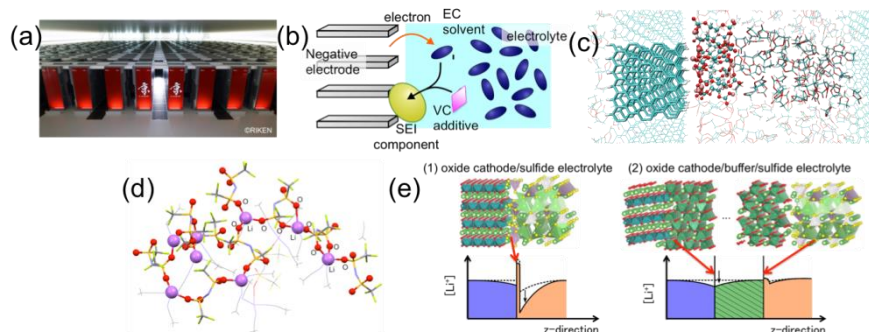
<sup>1</sup>WPI-MANA, NIMS, <sup>2</sup>ESICB, Kyoto Univ., <sup>3</sup>MI<sup>2</sup>I, NIMS

**Keywords:** DFT, free energy calculation, redox reaction, interfacial process

Search for batteries with better performance (larger energy density) and more reliability (more safety) has been extensively done by lots of researchers for decades. However, the atomistic mechanisms of chemical (redox) reactions and ion transports have not been fully understood yet, because of the difficulty in the in-situ measurements.

In order to address these issues, we have developed a well-parallelized and –optimized DFT free energy calculation code, based on an open code “CPMD” maintained by IBM Zurich. Then, we have carried out highly-accurate and –efficient DFT simulations on the K (10<sup>16</sup> Flops) computer, world no.4 at the moment (Fig.(a)).

We found a novel mechanism of the VC additive effect on the reductive decomposition of EC solvent (Fig.(b)), and proposed a probable subsequent mechanism for formation of solid electrolyte interphase (SEI) layer at the electrolyte-electrode interface (Fig.(c)). We also elucidated origins of the unusual redox stability and ion transport in a new concept of superconcentrated electrolytes (Fig.(d)). On the interfacial resistance between oxide cathode - sulfide electrolyte, we demonstrated that Li ion depletion can play an important role (Fig.(e)). These findings have provided a new perspective on battery science.





## Corsin Battaglia

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### Previous Positions

2012-2014 Postdoc at University of California Berkeley & Lawrence Berkeley Laboratory

2009-2011 Postdoc at Ecole Polytechnique Fédérale de Lausanne

2004-2008 PhD at Université de Neuchâtel

### Research Interests (Several lines)

Empa's laboratory Materials for Energy Conversion strives to solve industry-relevant challenges for sustainable energy conversion and storage technologies through materials and device innovation. Our research aims at developing fundamental knowledge through experiment and modelling enabling materials and processes that improve performance, cost, and reliability of batteries, electrolysis, photovoltaics and thermoelectrics.

### A new class of solid-state electrolytes for lithium ion batteries with conductivities near liquid electrolytes

Yigang Yan<sup>1</sup>, Ruben-Simon Kühnel<sup>1</sup>, Arndt Remhof<sup>1</sup>, Daniel Rentsch<sup>1</sup>, Zbigniew Lodziana<sup>2</sup>, Corsin Battaglia<sup>1</sup>

<sup>1</sup> Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland

<sup>2</sup> Institute of Nuclear Physics, Polish Academy of Sciences, Poland

**Keywords:** *Lithium ion batteries, solid-state electrolytes, ion conductivity*

Solid-state electrolytes offer potentially improved operational safety for lithium ion batteries. Especially at lower temperatures (at or near room temperature), most solid-state electrolytes display lithium ion conductivities lower than the one of conventional organic liquid electrolytes limiting output power. Several sulfides are among the only compounds reported so far displaying lithium ion conductivities in the range of liquid electrolytes. However, guaranteeing thermal and/or electrochemical stability of sulfide electrolytes remains challenging.

Here we report several complex hydrides that display, for the first time, lithium ion conductivities near room temperature comparable to liquid organic electrolytes, adding a second class of materials to the group of highly conductive solid state electrolytes and paving the way for high-power lithium solid-state batteries. An in depth study was carried out to understand the lithium transport mechanism of these materials. Density functional theory calculations combined with molecular dynamics simulations support a new anion assisted lithium hopping mechanism. We also show excellent stability of our solid state electrolyte via long-term cycling in half-cell battery configuration.



## Michihisa Koyama

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### Previous Positions

2003.10-2008.11 Assistant Professor, Tohoku University

2002.4-2003.9 Postdoctoral Fellow, The University of Tokyo

### Research Interests

- Practical application of computational chemistry to energy devices
- Fuel cell
- Lithium ion battery
- Nano-alloy for heterogeneous catalysis
- Scenario design of future energy systems

## Multi-Physics Simulation of Porous Electrode for Lithium Ion Battery

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<sup>2</sup> International Institute for Carbon-Neutral Energy Research, Kyushu University

**Keywords:** Multi-Physics Simulation, Lithium Ion Battery, Porous Electrode

In the porous electrodes of lithium ion battery (LIB), physics such as charge-transfer reactions, diffusion, and conduction concurrently proceeds in a highly coupled manner. Thus, tuning the microstructure to provide better paths for involved species as well as increase active sites for reactions is of great importance. In author's research group, multi-physics simulation method for LIB electrode is ongoing [1]. The developed method and its application will be introduced.

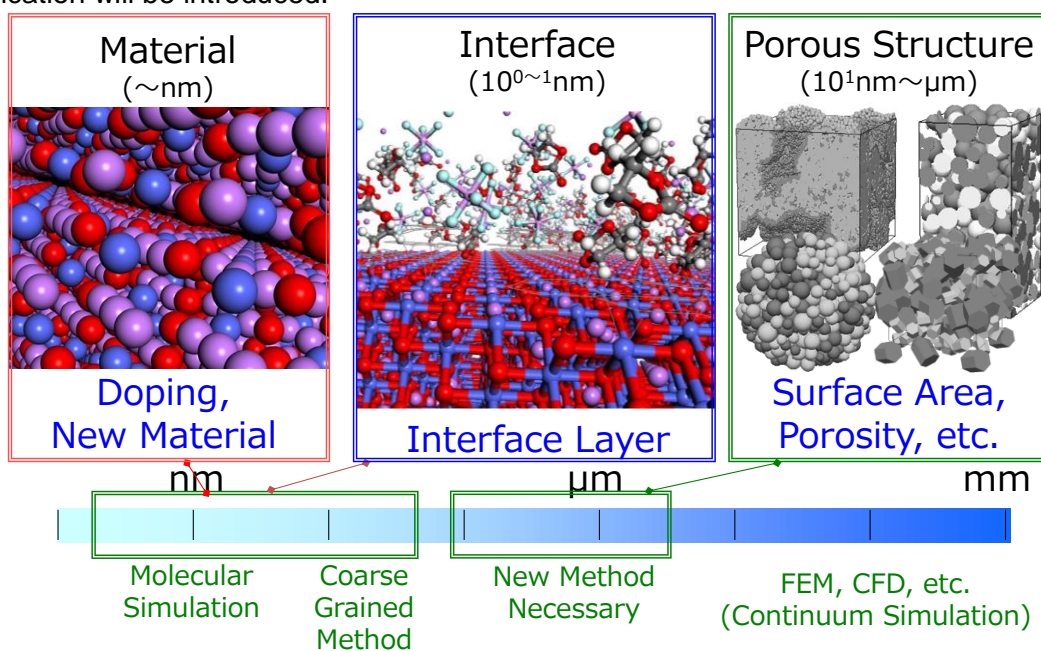


Fig. 3 Design Approaches for Porous Electrode System in Energy Devices



## Satoshi Horike (*Poster only*)

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### Previous Positions

2007-2009 Postdoctoral fellow, UC Berkeley

2011-2015 Researcher, JST PRESTO

### Research Interests

Solid state ionics, coordination chemistry, glass, fuel cell/battery materials

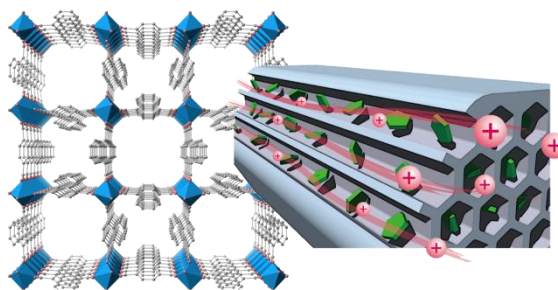
## Anhydrous proton conductive metal organic frameworks for fuel cell technology

Satoshi Horike

Graduate School of Engineering, Kyoto University

**Keywords:** Proton conductor, metal organic framework, glass

Solid state ion conductors are significant class of materials for battery, fuel cell, electrocatalysis, and sensor. General challenges are how to have fast ion conductivity with wide working temperature range, and how to handle the materials' mechanical properties and morphology for device integration. To approach these issues, we focus on metal organic frameworks (MOFs) consist of metal ions and bridging ligands (Figure).<sup>1</sup> MOFs have ordered arrangement of functional groups, and for example, the optimized hydrogen bond networks in the frameworks offer anhydrous H<sup>+</sup> conductivity (over 10<sup>-2</sup> S cm<sup>-1</sup> at above 100 °C) which is a big demand for fuel cell vehicle technology. In addition to the beneficial designability in molecular scale, some ion conductive MOF crystals show melting behavior or transformation of glassy state by thermal/mechanical treatments.<sup>2,3</sup> The phase transitions enables to fabricate variety of materials morphology such as thin film, fiber, and composites. The organic/inorganic hybrid nature of MOF material for solid state ionics will be discussed.



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2. D. Umeyama, S. Horike, M. Inukai, T. Itakura and S. Kitagawa, *J. Am. Chem. Soc.*, 2015, **137**, 864-870.
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### **Previous Positions**

2003-2007 Research Associate, Central Research Institute of Electric Power Industry

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### **Research Interests**

Electrochemistry, Solution Chemistry, Materials Sciences

## **Ionic Liquids as Electrolyte Materials for Energy Storage / Conversion Devices**

### Shiro SEKI

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**Keywords:** *Ionic Liquid, Lithium Battery, Capacitor, Organic-FET*

Room-temperature ionic liquids (RTILs) have many desirable physical and chemical properties required for electrolyte materials of energy conversion and storage device owing to their low-flammability, low-volatility, high ionic conductivity, and high thermal stability. Recently, we are promoting research and development of RTILs as electrolyte materials for lithium secondary batteries, electric double layer capacitors (EDLCs), and organic field effect transistors (OFETs). For achieving high performance (long-life, high capacity / power) electrochemical devices, intrinsic understanding of physicochemical properties for RTILs is very important. In particular, molecular combinations of RTILs (cations and anions), for example, frameworks, main elements, and substituent groups are very important factors. In this presentation, I will report following two topics concerning from basic to application for RTILs.

#### 1. Physical and chemical properties of RTILs

Chemical structures of RTILs (cations and anions) have an impact on the macroscopic physical properties (viscosity, density, ionic conductivity, self-diffusion coefficient). In particular, I will report general / specific physicochemical properties of RTILs.

#### 2. Electrochemical applications of RTILs

Necessary physicochemical properties of RTILs changes depending on the various electrochemical devices (lithium batteries: specific insolubility, electrochemical stability, viscosity, EDLCs: viscosity, ionicity, affinity with electrodes, OFETs: viscosity, carrier density, affinity with electrodes, and so on). I will discuss about the relationships between RTIL species and performances of various electrochemical devices such as lithium secondary batteries (including lithium-sulfur batteries), EDLCs, and OFETs.





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### Previous Positions

2003-2005 Research Scientist, National Institute of Advanced Industrial Science and Technology (AIST)

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2007-2009 Assistant Professor, Tokyo University of Science

2009-2012 Associate Professor, Doshisha University

### Research Interests

Li-air batteries, Li-ion batteries, Capacitors and Fuel cells

### Ion Transport Analysis on Glyme-based Electrolyte Solutions for Li-air Batteries

Morihito Saito<sup>1</sup>, Shinya Yamada<sup>1</sup>, Kimihiko Ito<sup>2</sup> and Yoshimi Kubo<sup>2</sup>

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**Keywords:** *Li-air batteries, Electrolyte solutions, Ion Transports, PGSE-NMR*

In order to clarify the Li<sup>+</sup> ion transport in glyme-based electrolyte solutions for Li-air batteries, LiCF<sub>3</sub>SO<sub>3</sub>(LiTfO) or LiN(SO<sub>2</sub>CF<sub>3</sub>)<sub>2</sub>(LiTFSI) dissolved glyme (triglyme(G3), tetra- glyme(G4) and pentaglyme(G5)) electrolytes were prepared, and the self-diffusion coefficients *D* of Li<sup>+</sup> ion (<sup>7</sup>Li), anion (<sup>9</sup>F) and glyme (<sup>1</sup>H) solvent were measured individually by a pulsed-field gradient spin echo (PGSE-)NMR in the temperature range of 30°C to 60°C. The viscosity, density and ionic conductivity were also examined to analyse the mechanism of ion transport in the glyme-based electrolytes. Moreover, molecular dynamics (MD) simulation was conducted to reproduce the *D* values and investigate the solvation structure of Li<sup>+</sup> ion by the glyme solvents. As the results, it was found that the glyme with shorter polyethylene glycol (PEG) chains gave a higher *D* value owing the lower viscosity and LiTFSI salt exhibited higher dissociation in glyme solvents to make much amount of Li<sup>+</sup> carriers, which enhanced the  $\sigma$  value of LiTFSI-based electrolyts. The trend was kept in the examined temperature range from 30°C to 60°C. However, the degree of dissociation ( $\alpha$ ) for the Li salts was decreased by an increase in the temperature, implying a reduction of the interaction energy between the Li<sup>+</sup> ion and glyme solvents to make a metal complex. On the other hand, the  $\alpha$  value was increased by the concentration of both Li salts in the electrolytes up to the molar ratio of 1:1 although the viscosity was also increased. Consequently, the highest ionic conductivity was attained both for 1 M LiTfO and LiTFSI-based electrolytes. From the results of MD simulation, the above trend of *D* values for ions and solvents were clearly reproduced and the larger amount of ion pairs of LiTfO was also confirmed than those of LiTFSI in the glyme solvents. The distance between Li<sup>+</sup> ion and anion was much expanded for the LiTFSI compared with that for the LiTfO. Based on those results, we further investigated on the other new Li salt, LiN(SO<sub>2</sub>F)<sub>2</sub>(LiFSI), and influence of impurity such as H<sub>2</sub>O from air to the ion transports. The reports will be presented in the workshop.

This study was supported by JST “Next Generation Batteries Area in Advanced Low Carbon Technology Research and Development Program (ALCA)” from MEXT, Japan.



**Tuesday March 8**  
**Session 6**  
**Data Driven Design**



## Koji Tsuda

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Germany

2009-2013 Senior Research Scientist, AIST, Japan

2014 Professor, University of Tokyo

### **Research Interests**

Machine Learning, Materials Informatics, Computational Biology

## **Machine Learning for Materials Discovery: Virtual Screening and Bayesian Optimization**

Koji Tsuda<sup>1</sup>

<sup>1</sup> University of Tokyo

**Keywords:** *Machine learning, Experimental design, Materials discovery*

Machine learning-based design of experiments appears in many different contexts in chemistry and physics. The scientific process of discovering new knowledge is often characterized as search from a space of candidates, and machine learning can accelerate the search by properly modelling the data and suggesting which candidates to apply experiments on. In many cases, experiments can be substituted by first principles calculation. I review two basic machine learning techniques called virtual screening and Bayesian optimization for fast discovery. The power of this approach is exemplified by two of our recent studies. One is discovery of compounds of low lattice thermal conductivity from the materials project database (Seko et. al., PRL 2015) . The other is fast determination of atomic structure of a crystalline interface (Kiyohara et al., JJAP 2016).



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### Previous Positions

2003-2004 JSPS Research Fellow, Kyoto University

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2007-2008 JSPS Postdoctoral Fellow for Research Abroad, University of Oslo

### Research Interests

Solid State Ionics, First Principles Calculation, Point Defect, Interface, Diffusion, Ceramics

## First Principles Calculations of Diffusion and Defect Formation Mechanism in Solid State Ionic Conductors

Akihide Kuwabara<sup>1</sup>, Kohji Fujimura<sup>1,2</sup>, Atsuto Seko<sup>2</sup>, Craig A. J. Fisher<sup>1</sup>,  
Hiroki Moriwake<sup>1</sup> and Isao Tanaka<sup>1,2</sup>

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**Keywords:** Solid Electrolyte, Ionic Conductivity, First Principles Calculation

Solid electrolytes for solid state ionic devices such as batteries and fuel cells are key technology of electric power resources. Performance of the devices is mainly attributed to ionic diffusivity in solids. It is importance to understand defect formation behavior and diffusion mechanism in the devices.

**[Li-ion conductor]** Toward the development of next-generation all solid rechargeable batteries, it is essential to further improve ionic conductivity of solid electrolytes. LISICON is a solid solution system of  $\text{Li}_{2+2x}\text{Zn}_{1-x}\text{GeO}_4$  ( $0 \leq x \leq 1$ ) and is one of the classical  $\text{Li}^+$  ion conductors. In this work, diffusion behavior of  $\text{Li}^+$  ions in LISICON-based ionic conductors was studied by first principles molecular dynamics (FPMD) simulations. From analysis of trajectory for  $\text{Li}^+$  ions, we found Li-ion diffusion via an interstitialcy mechanism. In this mechanism, excess  $\text{Li}^+$  ion at an octahedral site jumps to a tetrahedral site and the  $\text{Li}^+$  ion at the tetrahedral site simultaneously jumps to another octahedral site.

**[Proton conductor]** Acceptor-doped  $\text{BaZrO}_3$  shows high proton conductivity under wet atmosphere conditions and is a promising material used as a proton conductive electrolyte of a solid oxide fuel cell. Similar to other kinds of ionic conductors, however, carrier trapping by dopant occurs and suppresses protonic conductivity. In this work, we calculate association energies between acceptors and protons in  $\text{BaZrO}_3$  using first principles calculations. Several types of cations, Sc, In, Lu, Y, Er, Gd and Eu, are adopted as acceptors for comparison. From the series of our calculations, it is revealed that dopants can be categorized into two types. In the cases of dopants with smaller ionic size such as Sc, In and Lu, protons prefer to be located at the first nearest neighbor from the dopants. Cations with larger ionic size like Y, Er, Gd and Eu capture protons at the next nearest neighbor sites.



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### Previous Positions

2008-2015 Research Staff Member, IBM Research Zurich

Research Interests (Several lines)

In the past years, I have led research activities on algorithmic developments for QM/MM, NDDO, DFT and molecular dynamics simulations. I have contributed as one of the main developers of the CP2K and CPMD packages. Currently, my interest is focused on developing mathematical kernels for large-scale electronic structure simulations, GPU acceleration and in combining cognitive computing to molecular modeling activities for predicting novel materials.

### Cognitive design of novel solid state electrolytes

M. Mottet, I. Tavernelli, T. Laino, C. Bekas and P. Staar  
IBM Research - Zurich, CH-8803 Rüschlikon

**Keywords:** *Material design, Cognitive Computing, Molecular Modeling*

Solid state electrolytes (SSEs) are inorganic materials that conduct ions at room temperature with mobilities close to the ones of liquid electrolytes, having - in addition - other properties such as electrochemical stability against the anode and cathode, and environmental stability so to reduce the complexity of batteries. Because of these properties, SSEs can potentially replace conventional organic solvents, which are flammable and toxic, thus to drastically improve the operational safety of the battery and, by inhibiting the dendrite growth, allowing the use of metals as anodes. This in turn increases the cell voltage and thereby increases the energy density of the battery. In the last decade, we experienced the discovery and characterization of a handful class of materials having high ionic conductivity at room temperature and low activation energy ( $E_a$ ) for use over a broad range of operating temperatures. Still, none of them meets all the required properties (conductivity, electrochemical stability, mechanical strength, etc.) to drive the novel battery technological innovation.

The discovery of new SSEs has largely proceeded by extending materials with desired properties into new compositional spaces. In this work we present a novel approach based on the use of cognitive computing technologies coupled to molecular modeling simulations to develop specific criteria for screening and finally designing better SSEs. In this talk, I will present the basics of cognitive computing coupled to molecular modeling activities and the novel approach at the base of the new SSEs design process.



## Motoko Kotani

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### Previous Positions

1990-1997: Lecturer, Department of Mathematics. Faculty of Science, Toho University

1993-1994: Visiting Researcher, Max-Planck Society for the Advancement of Science

1997-1999: Associate Professor, Department of Mathematics. Faculty of Science,  
Toho University

1999-2003: Associate Professor, Mathematics Institute, Graduate School of Science,  
Tohoku University

2001.4-2001.11: Visiting Professor, Institute of Advanced Scientific Studies (IHES)

2004-present: Professor, Mathematics Institute, Graduate School of Science, Tohoku  
University

2008-2014.3: Distinguished Professor, Mathematics Institute, Graduate School of  
Science, Tohoku University

2011-2012: Deputy Director, Professor, WPI-AIMR, Tohoku University

2012-present: Director, AIMR, Tohoku University

### Research Interests

- Mathematics, Discrete Geometric Analysis in particular. Also interested in application to  
Materials Science, Condensed Matter Physics

## Mathematical Challenge to a New Phase of Materials Science

Motoko KOTANI

Advanced Institute for Materials Research

**Keywords:** *Structural Understanding, Topology, Discrete Geometric Analysis*

WPI-AIMR is one of the six institutes chosen by the MEXT to build a visible research center on the world scene under the World Premier International Research Center Initiative(WPI) program. AIMR's ultimate goal is to integrate materials science with physics, chemistry, engineering and mathematics to create a new materials science and contribute to society. More precisely, our mission is to conduct collaborative and interdisciplinary researches beyond conventional ideas along with the following objectives: (1)To elucidate fundamental principles lying behind functional manifestation common to different kinds of materials,(2)To build a basis for "predicting" new functions and new materials based on the newly-established principles,(3)To create Green Materials to contribute to "Energy Harvesting", "Energy Saving" and "Environmental Clean-up". Mathematics act as a catalyst to accelerate interdisciplinary research by providing a universal frame work. Last year, we set up three target projects: "Non-equilibrium Materials based on Mathematical Dynamical Systems", "Topological Functional Materials", "Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis". In the workshop, I will present some of emerging results under the scheme.

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**Previous Positions**

2010-2013 Post doctoral researcher, Department of Physics, Kyushu University

2013-present Assistant professor, WPI-AIMR Tohoku University

**Research Interests**

- Statistical mechanics, Computational complexity, quantum annealing, Machine learning

**Machine learning for recognizing rock texture : Toward automation of professional criteria**Chihiro Nakajima<sup>1</sup>, Masayuki Ohzeki<sup>2</sup><sup>1</sup>WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University<sup>2</sup>Department of Systems Science, Graduate School of Informatics, Kyoto University

An application of Boltzmann machine learning for an analysis of rock-textures by image segmentation based on semi-supervised learning is introduced. First, the CT images of a rock sample are prepared for non-destructive observation of the internal structure. The CT images are obtained as gray scale images of 256 gradations. In addition, these images contain noises and blurs. The texture of rock samples is composed of three kinds of domain; crystal, melt and void (bubbles of gas). Hence, one of the three-kind labels is assigned to each local region in the image. In terms of image processing, this task is regarded as image segmentation.

In the scene of mineralogy the precise protocol for this segmentation is established. However, this protocol requires complicated process and takes time. Thus it has not been able to fully utilize the CT-images as data.

We propose a method for automation of this segmentation protocol. The process of segmentation itself is implemented by Bayesian inference with appropriate probabilistic (generative) model. The generative model requires hyper parameters to be fixed. We determined the hyper parameters by Boltzmann learning from the small area processed with conventional protocol. With this framework the professional criteria of the label-assignment seems to be fairly successfully reproduced and the segmentation process is accelerated enough to utilize all data of CT-images.

The framework introduced in this study is expected to be effective for massive data processing, and automation the efficiency of skilled detection or diagnosis.



**Tuesday March 8**

**Session 7**

**Photocatalysis/Electrocatalysis/  
Catalysis B**



## Kenji Miyatake

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### Previous Positions

1995-1996 Research Associate, Waseda University, Japan

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1999-2001 Lecturer, Waseda University, Japan

1999-2001 JSPS Postdoctoral Fellow for Research Abroad, McGill University, Canada

2001-2009 Associate Professor, University of Yamanashi, Japan

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### Research Interests

polymer chemistry, fuel cells

### Molecular design, synthesis, and properties of anion exchange membranes for alkaline fuel cells

Kenji Miyatake

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**Key Words:** *fuel cells / anion conduction / membranes*

Alkaline fuel cells (AFCs) using anion exchange membranes are attractive energy devices for stationary, automotive, and mobile applications because of their high energy density, high conversion efficiency, and low pollution levels. The possible use of non-precious metals as electrocatalysts is a great advantage over proton exchange membrane fuel cells. However, the existing AEMs are not as conductive and stable as proton exchange membranes, which are major concerns in the development of high performance and durable alkaline fuel cells. In order to address the issues, a number of AEMs have been developed in the last decade. We proposed that the multiblock copolymers containing dense ammonium groups in the hydrophilic blocks are highly anion conductive due to distinct hydrophilic/hydrophobic phase separated morphology and interconnected ionic channels.<sup>1</sup> Aiming at even better performing AEMs, we have proposed a novel series of AEMs containing ammonium functionalized oligophenylene moieties as hydrophilic component.<sup>2,3</sup> The combination of the hydrophilic component with the perfluoroaliphatic chains provides ductile membranes with high hydroxide ion conductivity and reasonable alkaline stability. Detailed synthesis, chemical and physical properties, and precious metal free alkaline fuel cell performance are reported.

- 1) M. Tanaka, K. Fukasawa, E. Nishino, S. Yamaguchi, K. Yamada, H. Tanaka, B. Bae, K. Miyatake, M. Watanabe, *J. Am. Chem. Soc.*, 133, 10646-10654 (2011).
- 2) N. Yokota, M. Shimada, R. Akiyama, E. Nishino, K. Asazawa, J. Miyake, M. Watanabe, K. Miyatake, *Macromolecules*, 47, 8238-8246 (2014).
- 3) H. Ono, J. Miyake, S. Shimada, M. Uchida, K. Miyatake, *J. Mater. Chem. A*, 3, 21779-21788 (2015).



## Raffaella Buonsanti

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### Previous Positions

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2012-2013 Project Scientist at the Molecular Foundry at LBNL

2010-2012 Postdoctoral Researcher at the Molecular Foundry at LBNL

### Research Interests

The Laboratory of Nanochemistry for Energy focuses on the synthetic design of atomically defined materials and their implementation into proof-of-concept energy devices to build unambiguous structure/property relationships so to guide the development of better performing materials in energy applications. Our current interest is converting CO<sub>2</sub> and water into fuels; we are developing fundamental understanding to “turn trash into treasure”.

### Colloidal Chemistry to advance solar-to-fuel conversion studies

Raffaella Buonsanti<sup>†</sup>

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**Keywords:** *nanocrystals, new materials, water splitting, CO<sub>2</sub> electrochemical reduction*

When aiming at maximizing performance of energy devices, the ability to tailor-make material platforms with tunable morphological characteristics in an unrestricted compositional range is critical for achieving optimal design specifications, as well as for providing understanding of the sensitivities of performance parameters to different compositional and structural parameters.

Colloidal synthesis is a surfactant-assisted approach that has proven to be one of the most powerful solution-based processes to tailor the size, the shape and the composition of nanocrystalline materials. This superior control afforded by colloidal chemistry, combined with solution processability and rich surface chemistry, has provided access to modular inorganic nanocomposites with an unprecedented tunability. Nonetheless, the full potential of colloidal chemistry has not yet been explored for solar-to-chemical energy conversion.

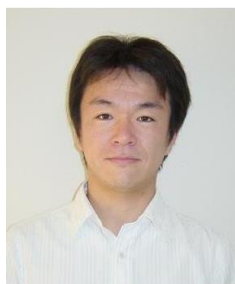
This talk highlights how colloidal chemistry can aid to construct materials for storing energy in chemical bonds. Specifically, our recent studies on complex metal oxide light absorbers to drive water oxidation and on metal catalysts to carry out electrochemical CO<sub>2</sub> reduction will be discussed.<sup>1-4</sup>

1. J. Lynch, C. Giannini, J. K. Cooper, A. Loiudice, I. D. Sharp, R. Buonsanti *J. Phys. Chem. C* **2015**, 119, 7443.

2. A. Loiudice, J. Ma, W. S. Drisdell, T. M. Mattox, J. K. Cooper, T. Thao, C. Giannini, J. Yano, L.-W. Wang, I. D. Sharp, R. Buonsanti *Adv. Mater.* **2015**, 27, 6733.

3. A. Loiudice, J.K. Cooper, Lucas H. Hess, T.M. Mattox, I.D. Sharp, R. Buonsanti *Nano. Lett.* **2015**, 15, 7347.

4. A. Loiudice, P. Lobaccaro, E. Kamali, T. Thao, B. Huang, J. Ager, R. Buonsanti, *in preparation*.



## Shintaro Ida

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### Previous Positions

2005-2009 Assistant Professor; Kumamoto University

### Research Interests

Photocatalyst for water splitting, photoelectrochemical water splitting

### Nanosheet photocatalysts for water splitting

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**Keywords:** *Photocatalyst, Hydrogen, Nanosheet*

Hydrogen production from water using photocatalyst is an ultimate goal in a renewable energy research. However, there are several issues such as the quantum efficiency in visible light region is still low for the practical application. One factor that causes a decrease in the photocatalytic activity is a recombination reaction between electron and hole. When the photocatalyst is illuminated by light with a energy greater than the bandgap energy, the photo-excited electron and hole are generated within the power. For these carriers generated within the powder to react with water, they have to travel long distance to the surface from within. During the long trip to the surface, they may be recombined or get trapped at the defect sites. One of the ideal materials that can suppress the recombination and give short travel distance is a two-dimensional material without inner and surface defects. Specifically, two-dimensional crystal (nanosheet) prepared by exfoliation of layered compound is a single crystal with a homogeneous ultrathin thickness, and has a lateral dimension from several hundred nanometer to several micrometer. Therefore, the travel distance of the photo-excited carriers is short, and many photons can be absorbed by nanosheet in a remarkably short time under low photon flux density due to its large section area. In this study, we have focused on the characteristic performance of nanosheet photocatalysts. For instance, it is well known that a photocatalyst without co-catalyst loading has poor photocatalytic activity for water splitting. However, a particular type of oxide nanosheet shows a high photocatalytic activity for hydrogen evolution from water without co-catalyst loading. Thus, the two-dimensional structure is expected to contribute to the development of photocatalysts for water splitting in the future. In this presentation, we report the characteristic performance of nanosheet photocatalysts and nanosheet p-n junction photocatalysts. The nanosheet p-n junction has an ideal surface for understanding the carrier transfer during the photocatalytic reaction. In this system, the driving force of the carrier transfer to oxidation and reduction sites was found to be the potential gradient generated by the nanosheet p-n junction.



## Markus Niederberger

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### Previous Positions

2012 – present: Associate Professor, ETH Zurich

2007 – 2011: Assistant Professor, ETH Zurich

2002 – 2006: Group Leader (Max Planck Institute of Colloids and Interfaces, Potsdam)

### Research Interests

The research of the Laboratory for Multifunctional Materials is focused on the development of liquid-phase synthesis routes to inorganic nanoparticles, study of their crystallization and formation mechanisms by *ex-situ* and *in-situ* tools, their surface functionalization, and their assembly and processing into films and nanostructured bulk materials for applications in gas sensing, photocatalysis, photoelectrochemical water splitting and lithium ion batteries.

### **Nanoparticles as Building Blocks for 2- and 3-Dimensionally Structured Materials for Energy Applications**

Markus Niederberger<sup>1</sup>

<sup>1</sup>Laboratory for Multifunctional Materials, Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 5, 8093 Zurich, Switzerland

#### **Nanoparticles, metal oxides, thin films, aerogels, lithium ion batteries**

Nanostructures including nanoparticles, nanowires and nanosheets are the ideal building blocks for the bottom-up fabrication of functional materials. They offer an immense variety of interesting properties, which not only depend on the composition, but also on the crystal structure, the particle size and shape and on the surface chemistry. Accordingly, potential synthesis routes have to provide full control over all these parameters. In addition, for most applications the nanoparticles have to be assembled and processed into useful geometries, including 2-dimensional arrangements like films or 3-dimensional bodies like composites, foams or aerogels.

The talk will give a short introduction to the synthesis of metal oxide nanoparticles by nonaqueous sol-gel chemistry, which involves the reaction of molecular precursors such as metal halides, alkoxides, acetates or acetylacetonates with organic solvents in the temperature range of 50-250 °C. For further processing and assembly, the nanoparticles are surface-functionalized and dispersed in different solvents. 2D structures like films are fabricated by spin-coating or doctor-blading of nanoparticle dispersions, typically followed by a heat treatment, while 3D materials like aerogels are produced by controlled gelling of the nanoparticle dispersions and subsequent supercritical drying in CO<sub>2</sub>. Finally, several examples will be shown, how the films and aerogels are tested for specific applications in energy storage and conversion.



## Stephen Matthew Lyth

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### Previous Positions

- 2011 - 15 WPI Assistant Professor, I2CNER, Kyushu University, Japan
- 2008 - 11 Postdoctoral Researcher, Tokyo Institute of Technology, Japan  
Department of Organic & Polymeric Materials, School of Engineering

### Research Interests

Carbon; heteroatom-doped-carbon; nanostructured carbons; graphene; carbon nanotubes; electrochemistry; hydrogen production, storage, & utilization; CO<sub>2</sub> conversion, fuel cells.

### Heteroatom-doped Carbons for Electrochemical Energy Conversion

S. M. Lyth, J. Liu, A. Mufundirwa, T. Bayer, B. Cuning, B. Smid, M. Nishihara, & K. Sasaki  
*Kyushu University, Fukuoka, Japan*

We produce **carbon foam** at gram scale and surface area >2500 m<sup>2</sup>/g by decomposition of sodium ethoxide. In its undoped form, it has potential applications in **hydrogen storage**: a H<sub>2</sub> uptake of 2.6 wt% via physisorption at 77K is measured. The material is also an ideal Pt **catalyst support**, with high electrochemical surface area and impressive fuel cell performance. Heteroatom doping can be performed by changing the precursors. By decomposing “amino-ethoxides”, **nitrogen-doped carbon foam** is produced. This is an effective **Pt-free electrocatalyst** in acid media, giving insight into the oxygen reduction reaction in metal-free catalyst systems. In alkaline media, the activity is comparable to Pt, and negligible degradation occurs over 60,000 potential cycles, far out-performing Pt. By decomposing “fluoroethoxides”, superhydrophobic **fluorinated carbon** nanospheres are produced, which can be printed or sprayed onto arbitrary substrates. These are applied in electrolysis and fuel cell gas diffusion layers in order to improve water management. **Graphene oxide** can be formed into extremely strong membranes with extremely **low hydrogen permeability**, and promising **proton conducting properties**. Therefore we explore this material as a fuel cell membrane. Finally, **sulfonated graphene** has increased proton conductivity compared with graphene oxide, improving the **fuel cell** performance.

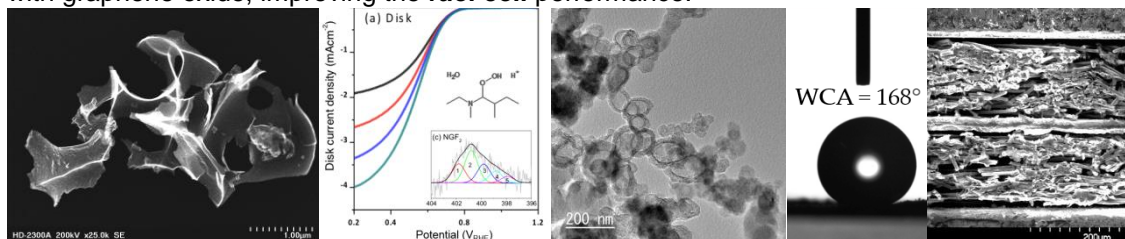


Figure: TEM image of our carbon foam; oxygen reduction reaction on nitrogen-doped carbon foam; superhydrophobic fluorinated carbon spheres; graphene oxide membrane fuel cell.



## Matthias Koebel

**Head Building Energy Materials & Components Laboratory,  
Swiss Federal Laboratories for Materials Science &  
Technology**

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### Previous Positions

2006-2014, Scientist & group leader, Empa Building Science & Technology Laboratory

2004-2006, Postdoctoral fellow, University of California, Berkeley, with Prof. G. A.

Somorjai

### Research Interests

- Porous materials, surface & interface science, materials chemistry, catalysis
- Aerogels, sol-gel materials, hybrid materials, nanocomposites
- Metal oxides, carbons, resin & other polymer chemistries, doping with various elements
- Lab-to market, scaleup, industrial process engineering

### Custom-tailored Carbon Materials for Energy Upgrading & Conversion

Lukas Huber, Shelly Arreguin, Michele Carboni and Matthias M. Koebel  
Empa, Swiss Federal Laboratories for Materials Science and Technology

**Keywords:** *Carbons, microporous, doping, hierarchical porosity, sorption cooling, electrochemistry*

In the upcoming transition phase from a fossil based energy economy to a renewable one, the quest for improved capture and conversion efficiency is primarily limited by materials properties and economic factors. Synthetic carbons are a class of materials with a tremendous potential for a variety of applications in renewable energy technologies. The main limitations of today's commercial carbons are their lack of i) structural (pore architecture) and ii) chemical (doping) control. Our laboratory is developing novel resin and polymer-based carbon materials with improved control of both, porosity and surface chemistry through bottom-up sol-gel processes. The resulting carbon materials toolbox employs low-cost fabrication processes, giving access to various morphologies such as films, powders and monoliths. A brief overview of synthetic methods and materials characterization tools / results will be presented.

From an energy conversion technology perspective, carbon materials are commonly used electrode materials in electrochemical storage (batteries / supercaps) and conversion systems (e.g. PEMFC). More recently, custom tailored carbons have also found interest as sorbents for upgrading thermal energy in the form of waste heat for heating and cooling applications by means of adsorption heat pumps. A quick overview of electrochemical storage and thermally driven heat pump research will be complemented by an outlook on further research challenges and opportunities for next generation carbon composite materials.



**Miho Yamauchi** (*Poster only*)

**Associate Professor, Kyushu University**

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**Previous Positions**

2008-2011 Associate Professor, Hokkaido University

**Research Interests**

Her research interests involve hydrogen related properties of metal and alloy nanoparticles, selective catalysis on the structure controlled nanoalloy catalysts and materials development for efficient energy conversion.

**Materials Development for the Realization of Carbon-Neutral Energy Cycles**

Miho Yamauchi<sup>1</sup>

<sup>1</sup> International Institute for Carbon-Neutral Energy Research, Kyushu University

**Keywords:** *Electrocatalyst, Energy carrier, Alcohol, Hydrogenation, Carboxylic acid*

The CO<sub>2</sub> concentration of the atmosphere has been inadvertently increased by consuming finite energy resources of fossil fuels, and increased concerns about climate issues due to CO<sub>2</sub> emissions have spurred the development of alternative and sustainable energy cycle systems. We have proposed novel energy cycles where electrical power is generated by partial oxidation of alcohols without CO<sub>2</sub> emission, and fuels are regenerated from oxidized wastes by using renewable energies, resulting in CO<sub>2</sub>-free power circulation, i.e., carbon-neutral energy (CN) cycles (Fig. 1).

We herein demonstrate the successful synthesis of a well-mixed Fe-group nanoalloy (NA) catalyst, a carbon supported FeCoNi NA catalyst (FeCoNi/C), that exhibits selective ethylene glycol (EG), a divalent alcohol, electrooxidation to oxalic acid (OX) without CO<sub>2</sub> emission in alkaline media.<sup>1</sup> Furthermore, an alkaline fuel cell fabricated with the FeCoNi/C anode catalyst and a solid oxide electrolyte was found to exhibit power generation from EG without any precious-metal catalysts.

Renewing alcoholic compounds by direct electroreduction of OX is another challenge, which enables highly efficient electric power circulation. To the best of our knowledge, the electroreduction of carboxylic acids to alcoholic compounds has never been achieved. We could demonstrate OX electroreduction into glycolic acid, an alcoholic compound, with significantly high selectivity (>98%) using pure anatase-type titania spheres under mild conditions.<sup>2</sup> These results are the first demonstration of a CO<sub>2</sub>-free electric power circulation using carbon containing compounds.

1. T. Matsumoto et al, *Sci. Rep.* **2014**, 4, 5620.

2. R. Watanabe et al, *Energy Environ. Sci.* **2015**, 8, 1456-1462.

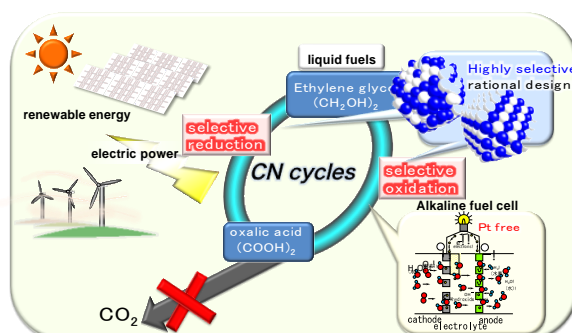


Fig. 1. Schematic image of carbon-neutral (CN) energy cycles.





## Akari Hayashi (*Poster only*)

**Professor / International Research Center for Hydrogen Energy, Kyushu University**

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### Previous Positions

2011.4 – 2015.3 Associate Professor at Kyushu University

2010.1 – 2011.3 Assistant Professor at Nagoya Institute of Technology

### Research Interests

Electrochemistry, electrocatalyst, carbon nanomaterial

More particularly, electrocatalytic reactions at fuel cells and electrolyzers are recent research interests.

### Development of PEFC cathode catalysts and investigation of their degradation mechanism

Akari Hayashi

International Research Center for Hydrogen Energy, Department for Hydrogen Energy Systems, WPI-I2CNER, and NEXT-FC at Kyushu University

**Keywords:** *Fuel cell, cathode, oxygen reduction, carbon corrosion*

Since commercialization of fuel cell vehicles (FCVs) started, realization of Hydrogen energy society has been accelerated. Even though they are now commercially available, increased efficiency is desired for further developing FCVs. Electrocatalysts for PEFC have an import role to govern FCV performance and are commonly made by Pt nanoparticles dispersed on carbon. Not only activity but also durability is required for next generation electrocatalysts.

In order to check long-term durability of electrocatalysts, development of accelerating degradation tests is necessary. In this study, we have developed a method to accelerate degradation using Environmental TEM (Hitachi HF-3300). Since carbon oxidation is one problem for cathode catalysts, real-time observation of Pt deposited carbon is performed under the oxidizing atmosphere thought the air introduction into the specimen chamber. Further, the specimen holder is heated up to 200 °C to accelerate carbon oxidation. In this system, both surface and transmitted images can be analyzed at the same position through simultaneous SEM and STEM observation.

By using this method, a new phenomenon of Pt particles embedded into carbon with almost no agglomeration has been observed. In order to investigate a possible mechanism of Pt embedding, carbon surface properties of electrocatalysts and also atmospheres within the chamber are controlled. As a result, on the graphitized carbon surface, Pt embedding is suppressed. When the same observation is performed under hydrogen atmosphere instead of air, Pt embedding phenomenon is not seen. Therefore, the mechanism of Pt embedding can be explained by accelerated carbon corrosion in the presence of Pt nanoparticles. The carbon under the Pt nanoparticles is corroded, leading to digging carbon surface and finally to embedding of Pt nanoparticles.

# General Information

## Hotel

### Sorell Hotel Sonnental

Zürichstrasse 94/96  
 8600 Dübendorf  
 T +41 44 802 12 82  
 sonnental@sorellhotels.com  
 www.sorellhotels.com/sonnental

## Airport transfer

From Airport to the Hotel **by tram**:

Take tram line **no. 12** in direction „Bahnhof Stettbach“.

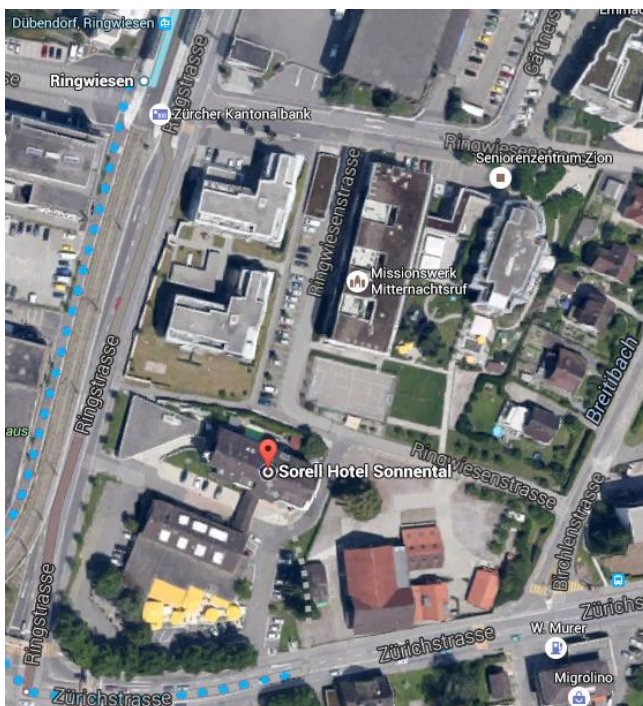
Get off at tram stop “Ringwiesen”. Walk along “Ringstrasse”.

After about 200 meters you reach Sorell Hotel Sonnental, Zürichstrasse 94/96.

[http://www.stadt-](http://www.stadt-zuerich.ch/vbz/en/index/timetables/online_timetable.html?S=Z%25C3%25BCrich%252C+Flughaven&Z=D%25C3%25BCbendorf%252C+Ringwiesen&date=06.03.2016&time=12%253A00&timesel=depart&submit=Search+connection)

[zuerich.ch/vbz/en/index/timetables/online\\_timetable.html?S=Z%25C3%25BCrich%252C+Flughaven&Z=D%25C3%25BCbendorf%252C+Ringwiesen&date=06.03.2016&time=12%253A00&timesel=depart&submit=Search+connection](http://www.stadt-zuerich.ch/vbz/en/index/timetables/online_timetable.html?S=Z%25C3%25BCrich%252C+Flughaven&Z=D%25C3%25BCbendorf%252C+Ringwiesen&date=06.03.2016&time=12%253A00&timesel=depart&submit=Search+connection)

<b>Tram fare:</b>	1-2 zones	1 hour	CHF 4.30	Single way
	1-2 zones	24 hours	CHF 8.60	Ticket is also valid for travelling to the City Center for 24 hrs

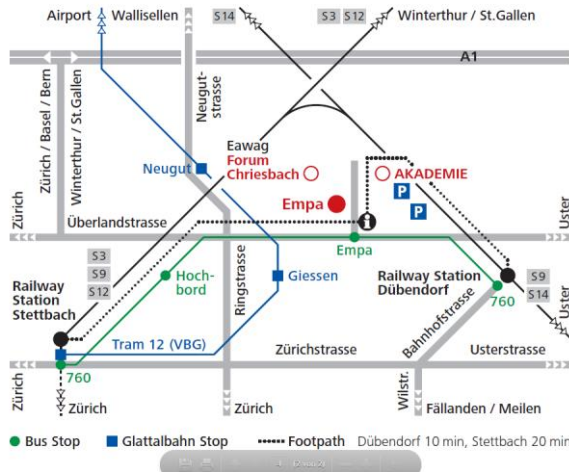


From Airport to the Hotel **by Taxi**:

The journey takes 10-15 minutes. Taxi fare about CHF 50.00

## Conference venue

Empa Akademie  
Überlandstrasse 129  
8600 Dübendorf



The conference venue is walking distance to the hotels or can be reached by tram (1 stop only). We will organize a group transfer.

## Conference Dinner, March 7, 2016

A group transfer will be organized from the conference venue.

Restaurant Saal / Hotel Bahnhof  
Bahnhofstrasse 64  
8600 Dübendorf  
+41 44 822 02 82  
<http://www.saal.ch/saal-restaurant-bar.php>

## Sightseeing City of Zurich and Dinner, March 8, 2016

Group transfer will be organized; Meeting point: Hotel Sonnentall Lobby, 5:45 pm

## Emergency contact numbers

Rahel Byland           +41 79 713 92 77  
Lucia Arpagaus       +41 79 760 49 90

