# 2019 International Symposium on Resource Chemistry

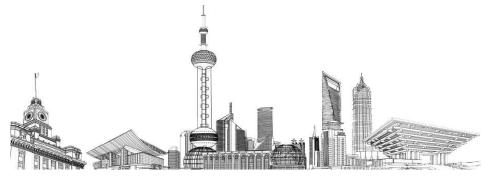
# **Shanghai Normal University**

May 14-16, 2019, Shanghai, China

**Supported by Chinese Chemical Society** 

**Chairman: Dieqing Zhang and Hexing Li** 





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# May 14, 2019

8:00-8:20 Registration, Room 126, Building 8, West part of SHNU

8:20-8:30 Room 126, Building 8, West part of SHNU

Chair: Prof. Dieqing Zhang, Shanghai Normal University

Opening Address: Prof. Ye Li, vice president of Shanghai Normal University

8:30-10:10 Lecture Section 1, Room 126, Building 8, West part of SHNU

Chair: Prof. Dieqing Zhang, Shanghai Normal University

**8:30-9:15 PL-1, Prof. Yunfeng Lu,** The University of California Los Angeles

Life is Good: a Journey from Energy Storage to Protein Therapeutics

**9:15-10:00 PL-2 Prof. Wonyong Choi,** Pohang University of Science and Technology (POSTECH)

Solar Production of H<sub>2</sub>O<sub>2</sub> through Selective Two-Electron Reduction of O<sub>2</sub>

10:00-10:10 Break, Room 126, Building 8, West part of SHNU

10:10-11:40 Lecture Section 2, Room 126, Building 8, West part of SHNU

Chair: Prof. Jian Zhu, Shanghai Normal University

**10:10-10:55 PL-3, Prof. Yusuke Yamauchi,** The University of Queensland, Australia, National Institute of Materials Science (NIMS), Japan Central China Normal University

Mesoarchitectonics: Inorganic Porous Materials

10:55-11:40 PL-4, Prof. Kirk Schanze, University of Texas at San Antonio

Photocatalysis Mechanisms and Polymer Chromophore-Catalyst Assemblies

12:00-13:40 Lunch, Taoliju Restaurant, SHNU

14:00-16:00 Academic committee member and consulting member meetings, Meeting Room 3 & 4, Conference Center, SHNU(Attendees: All the committee members and invited speakers)

15:00-17:40 Lecture Section 3, Room 126, Building 8, West part of SHNU

Chair: Dr. Xiaoyan Liu, Shanghai Normal University

**15:00-16:00 Prof. Kirk Schanze**, Editor-in Chief of ACS Applied Materials & Interfaces,

Introduction of how to prepare research paper

16:10-16:55 PL-5, Prof. Sang-Eon Park (朴尙彦), Inha University, Incheon, South Korea

Green Chemistry by Nanoporous Catalysts: Microwave Synthesis, Organofunctionality & Hierarchy

**16:55-17:40 PL-6, Prof. Yongfa Zhu,** Tsinghua University, China Supramolecular Photocatalyts for Pollutant Degradation and Tumor Removal

18:00-19:30 Dinner, Taoliju Restaurant, SHNU

# May 15, 2019

8:30-10:15 Lecture Section 4, Room 126, Building 8, West part of SHNU

Chair: Prof. Guisheng Li, Shanghai Normal University

**8:30-9:15 PL-7, Prof. Zhonglin Wang**, Chinese Academy of Sciences, Beijing, China; Georgia Institute of Technology, Atlanta, Georgia USA

The Physics of Contact-Electrification and Its Implication to New Energy Science

9:15-10:00 PL-8 Prof. Lianzhou Wang, The University of Queensland, Australia

Semiconductor Nanomaterials for Photoelectrochemcial Water Splitting

10:00-10:10 Break, Room 126, Building 8, West part of SHNU

10:10-11:40 Lecture Section 5, Room 126, Building 8, West part of SHNU

Chair: Prof. Yuning Huo, Shanghai Normal University

**10:10-10:55 PL-9 Prof. Steven L. Bernasek**, Yale-NUS College Singapore; Princeton University

Investigating Environmental Catalysis using the Tools of Surface Science

**10:55-11:40 PL-10 Prof. Gerd Buntkowsky,** Technical University Darmstadt, Germany Solid-State-NMR Characterization of functional Materials

11:50-13:30 Lunch, Taoliju Restaurant, SHNU

14:15-16:45 Acceptance Meeting of International Joint Laboratory on Resource Chemistry organized by the Ministry of Education of China Room 101, Meeting room of International affairs office, SHNU (Besides Foreign Guest Hotel)

# 14:15-14:30 Opening Ceremony (All guests)

**14:30-16:45 Checking Meeting** (Only Prof. Guoqin Xu and Prof. Andrew Bocarsly attend. Other professors please move to the 2<sup>nd</sup> floor meeting room of International affairs office)

# 14:35-15:35 Round-table talk with editor

2<sup>nd</sup> floor, Meeting room of International affairs office, SHNU (Besides Guest Hotel)

**Dr. Muxian Shen**, Editor of Willey Journals Introduction of Willey Journals

15:35-16:05 Research talk of the International Joint laboratory on Resource Chemistry 2<sup>nd</sup> floor, Meeting room of International affairs office, SHNU (Besides Guest Hotel)

Prof. Qinghai Deng, Shanghai Normal University

Non-precious metals catalyzed dearomatization

# **16:05-16:35 Pin Lv,** Shanghai Normal University

Self-driven ROS (Reactive Oxygen Species) Generation from the Intrinsic Property of Oxygen Vacancies

# 16:35-17:00 Prof. Zhenfeng Bian, Shanghai Normal University

Discussion on the publication of a special issue (Elsevier)

# 17:30-19:30 Dinner, Taoliju Restaurant, SHNU

# May 16, 2019

8:30-10:00 Lecture Section 6, Room 126, Building 8, West part of SHNU

Chair: Prof. Shengxiong Xiao, Shanghai Normal University

8:30-9:15 PL-11 Prof. Andrew Bocarsly, Princeton University, USA

New Metal Alloy Electrocatalysts for the Reduction of CO<sub>2</sub> to Multi-CarbonProducts

**9:15-10:00 PL-12, Prof. Michael S. Wong,** Rice University, Houston, TX, United States.

Water Upgrading Chemistry Using Precious Metal Catalysis

10:00-10:10 Break, Room 126, Building 8, West part of SHNU

10:10-11:40 Lecture Section 7, Room 126, Building 8, West part of SHNU

Chair: Prof. Zhenfeng Bian, Shanghai Normal University

10:10-10:55 PL-13, Prof. László Kürti, Rice University, Houston, USA

Practical & environmentally friendly nitrogen-transfer processes

10:55-11:40 PL-14, Prof. George A. O'Doherty, Northeastern University, Boston, MA

Furans as a practical chemical resource for oligosaccharides

11:50-13:30 Lunch, Taoliju Restaurant, SHNU

14:00-15:30 Lecture Section 8, Room 126, Building 8, West part of SHNU

Chair: Prof. Fang Zhang, Shanghai Normal University

**14:00-14:45 PL-15,Prof. Wei Wang,** University of Arizona, Tucson, USA; East China University of Science & Technology, China

C-C Bond Formation Enabled by Radical Engaged Organocatalysis

**14:45-15:30 PL-16, Prof. Quoqin Xu,** National University of Singapore, 10 Kent Ridge, Singapore

Design and Fabrication of Metal Oxide Semiconductors for Photocatalytic Applications

End of the symposium

# Life is Good: a Journey from Energy Storage to Protein Therapeutics

Yunfeng Lu

Department of Chemical and Biomolecular Engineering The University of California Los Angeles

Human civilization is associated with the harvest and utilization of solar energy. Driven by massive use of fossil fuels, the first industrial revolution (mainly driven by coal) and the second industrial revolution (mainly driven by oil) have established the modern civilization yet with ecological deterioration. Developing technologies that enable more effective energy harvest, storage and utilization has emerged as one of the most essential topics. In this presentation, I will discuss how to make electrochemical devices (e.g., supercapacitors, batteries, and fuel cells) with better performance, focusing on how to construct effective transport pathways for electrons and ions to facilitate the chemical transformations. Meanwhile, living organisms are made from the basic elements (e.g., C, O, H, N and P), consume energy and reproduce themselves through chemical transformations. In this context, life and energy are highly associated and the research on protein therapeutics will also be presented.

# Prof. Yunfeng Lu

# **Profession Preparation/Education**

Jilin University, China Chemistry B.S. 1991

Chinese Academy of Sciences Polymer Science M.S. 1994

The University of New Mexico Chemical Engineering Ph.D. 1998

Oct. 1998-Nov. 1999 Sandia National Laboratories

Nov. 1999-Dec. 2000 Senior Processing Engineer, Applied Materials, Santa Clara, CA

Jan. 2001 – July 2005 Assistant Professor, Tulane University

July 1, 2005 Sept. 2006 Brown Chair Professor, Tulane University

July 1, 2006 Present Professor of Chemical Engineering, UCLA

# **Major Honors and Awards**

- 1. Presidential Early Career Awards for Scientists and Engineers (PECASE)
- 2. Early Career Scientist and Engineer Awards, Department of Energy (DOE) (2005)
- 3. *Unilever Award*, American Chemical Society, Division of Colloid and Surface Chemistry (2005).
- 4. CAREER Award, National Science Foundation (2004)
- 5. Young Investigator Award, Office of Naval Research (ONR) (2003);
- 6. Victor K. LaMer Award, American Chemical Society (2000)
- 7. Outstanding Scientific Accomplishment Award, Department of Energy (DOE) Basic Energy Science (1998)

# **Grants and Funding**

Over several millions dollars funding supported by NSF, DOD, EPA, DOE, NIH, and industrial partner.

# **Book Chapters and Book Edited**

4 books and chapters published

#### **Publications**

Over 200 peer reviewed journal publications, including 11 in *Nature*, *Nature Nanotechnology*, *Nature Comm.*, and *Science*. Citation ~ 25,000, H-index ~ 71.

# **Patents and Provisional Patents**

Over 30 patents and patent applications

# **Supervision of Students and Post-docs**

Supervising 22 PhD students, 6 Postdocs.

# Solar Production of $H_2O_2$ through Selective Two-Electron Reduction of $O_2$

# Wonyong Choi

Division of Environmental Science and Engineering and Department of Chemical Engineering,
Pohang University of Science and Technology (POSTECH), Pohang 37673, Korea.

E-mail:wchoi@postech.edu

Photocatalytic and photoelectrochemical conversion of water, carbon dioxide, oxygen to useful chemicals and fuels is a promising solar conversion technology since it needs semiconductor materials and light only to carry out the catalytic reactions. The photocatalytic production of H<sub>2</sub>O<sub>2</sub> through dioxygen reduction has been receiving great attentions recently since it is an eco-friendly oxidant and fuel that generates water and dioxygen only as the reaction products. However, the low photoconversion efficiency hinders its practical application and expensive noble metals are usually needed as cocatalytic material. Here we report some successful examples of photocatalytic and photoelectrocatalytic systems which efficiently increase the production of H<sub>2</sub>O<sub>2</sub> through the selective two-electron transfer to dioxygen. Reduced graphene oxide/titania composites (rGO/TiO<sub>2</sub>), graphene oxide nanodisks (GONDs) attached to CdS-silica nanocapsules (SNCs) (GOND/CdS-SNC), graphitic carbon nitride photocatalysts modified with multi-component doping were prepared, characterized, and tested for their photoactivities of H<sub>2</sub>O<sub>2</sub> production. In particular, carbon nitride based photocatalysts are proposed as an ideal photocatalyst for the photosynthesis of H<sub>2</sub>O<sub>2</sub>. A photoelectrochemical cell in which H<sub>2</sub>O<sub>2</sub> is produced on both photoanode and cathode was also investigated and introduced. The present photocatalytic and photoelectrochemical systems consisting of earth-abundant elements only under visible light irradiation should make the solar production of  $H_2O_2$  more viable.

# **Prof. Wonyong Choi**

#### **Professor**

Division of Environmental Science & Engineering/ Dept. of Chemical Engineering Pohang University of Science and Technology (POSTECH), Pohang, Korea 37673

Phone: +82-54-279-2283 Fax: +82-54-279-8299

#### **Education**

1996. 6 **Ph.D.**, Chemistry (*Environmental Chemistry*)

California Institute of Technology (CALTECH), Pasadena, CA, U.S.A.

1990. 2 M.S., Chemistry (*Physical Chemistry*)

Pohang University of Science and Technology (POSTECH), Pohang, Korea

1988. 2 **B.S.** (with honors), Engineering (*Chemical Technology*)

Seoul National University (SNU), Seoul, Korea

# Professional Experience & Research Area

1998. 2 - present

**Professor**, Division of Environmental Science and Engineering/ Dept. of Chemical Engineering POSTECH

**Research area**: Semiconductor photocatalysis for environmental and energy applications; Solar hydrogen production; Development of visible light active photocatalysts; Advanced oxidation processes (AOPs); Developments of physicochemical methods for the destruction of recalcitrant pollutants; Environmental photochemistry and ice chemistry 1996. 6 - 1998. 2

**Postdoctoral Scholar**, NASA/Caltech Jet Propulsion Laboratory (JPL), *Atmospheric Chemistry Research Element, Earth and Space Sciences Division* 

**Research area**: Laboratory kinetic studies of heterogeneous atmospheric chemical reactions **Awards and Honors (Selected)** 

2018 Korea Engineering Award

2015 KAST Science and Technology Award

2014 Elected as Fellow of the Royal Society of Chemistry (FRSC)

2014 Elected as Fellow of Korean Academy of Science and Technology (KAST)

2012 Namgo (Jong-Ryul Lee) Chair Professor, POSTECH

2008 Lectureship Award for Asian and Oceanian Photochemist (*Japanese Photochemistry Association*)

2006 Young Scientist Award (Korean Academy of Science & Technology; Ministry of Science & Technology)

1988 Alumni Association President Award for Outstanding Engineering Students (SNU Engineering College)

# **Academic Achievements and Services (Selected)**

"291 research articles published in peer-reviewed journals (mostly in international SCI journals) with total citation >35,300 times, **H-index 78** (Web of Science, 2019/4), Google citation >47,800, H-index 89 (2019/4)

"Advised 23 Ph.D. and 27 M.S. degrees during the tenure of POSTECH (1998 - present) Associate Editor, Environ. Sci. Technol. (2017.4 - ); Editor, J. Hazardous Materials (2008.2 - 2017.3)

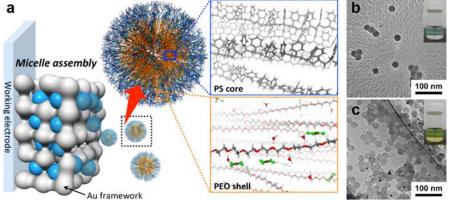
**Editorial board:** Energy Environ. Sci. (2008.5 - ), ACS Earth & Space Chemistry (2017.3 - ), Environ. Sci. Technol. (2015.2 - 2017.3), J. Phys. Chem. (2009.1 - 2011.12)

# **Mesoarchitectonics: Inorganic Porous Materials**

#### Yusuke Yamauchi

Professor, School of Chemical Engineering & AIBN, The University of Queensland, Australia Honorary Group Leader, National Institute of Materials Science (NIMS), Japan

Polymeric micelles are formed in solution when the hydrophobic portions are driven to an interior structure while hydrophilic portions are turned outward facing toward the water. Recently, we have focused on the polymeric micelles as stable and rigid templates for obtaining mesoporous materials with ultra large pore sizes. Our 'polymeric micelle assembly' approach is highly useful for preparation of novel mesoporous materials which are not easily obtained by general synthetic approaches. As one example, mesoporous gold (Au) films with tunable pores are expected to provide fascinating optical properties stimulated by the mesospaces, but they have not been realized yet because of the difficulty of controlling the Au crystal growth. Very recently, we reported a reliable synthesis of mesoporous Au films using stable micelles of polystyrene-block-poly(oxyethylene) (PS-b-PEO) diblock copolymers, with electrochemical deposition advantageous for precise control of Au crystal growth. In the electrolyte solution, HAuCl<sub>4</sub> is dissolved into H<sub>3</sub>O<sup>+</sup> and AuCl<sup>4-</sup> ions and then interacts with the EO shells of the micelles through hydrogen bonding. This interaction favours H<sub>3</sub>O<sup>+</sup> rather than AuCl<sub>4</sub>, and consequently creates positively charged micelles that can be directed to the working electrode surfaces, where the AuCl<sub>4</sub> ions are reduced to metallic Au with the electrochemical deposition of the micelles. The resultant mesoporous Au films actually exhibit high scattering performance and thus high activity for molecular sensing. Significantly, enhanced electric field (E-field) amplitude is clearly seen inside or at the perimeter of the mesopores. In this presentation, we would like to develop new mesoporous/nanoporous materials as well.



**Fig.** 1 | (a)

Schematic illustration for the fabrication of mesoporous Au films by using polymer micelle assemblies. (b, c) TEM images of PS-b-PEO micelles formed in aqueous solution (b) without and (c) with HAuCl<sub>4</sub> source. The Tyndall effect is also shown as an inset image.

Selected Publications in 2015-2018: J. Am. Chem. Soc., 140, 12434 (2018); Angew. Chem. Int. Ed., 57, 8881 (2018); Angew. Chem. Int. Ed., 57, 5848 (2018); Angew. Chem. Int. Ed., 57, 2894 (2018); Nature Commun., 8, 15717 (2017); Nature Commun., 8, 15581 (2017); Angew. Chem. Int. Ed., 56, 13508 (2017); Angew. Chem. Int. Ed., 56, 8435 (2017); Angew. Chem. Int. Ed., 55, 7836 (2017); Nature Chemistry, 8, 638 (2016); Angew. Chem. Int. Ed., 55, 10037 (2016); Angew. Chem. Int. Ed., 55, 8426 (2016); Angew. Chem. Int. Ed., 55, 8228 (2016); Angew. Chem. Int. Ed., 55, 12746 (2016); Angew. Chem. Int. Ed., 55, 12793 (2016); J. Am. Chem. Soc., 138, 13874 (2016); Nature Commun., 6, 6608 (2015); Angew. Chem. Int. Ed., 54, 951 (2015); Angew. Chem. Int. Ed., 54, 588 (2015); J. Am. Chem. Soc., 137, 11558 (2015); J. Am. Chem. Soc., 137, 1572 (2015).

# Prof. Yusuke Yamauchi

#### **Professor (Tenure)**

School of Chemical Engineering, The University of Queensland

E-mail: <u>y.yamauchi@uq.edu.au</u>

# **Education History:**

## April 1999 - March 2003

B.Eng., Department of Applied Chemistry, School of Science and Engineering, Waseda University

# April 2003 - March 2004

M.Eng., Department of Nanoscience & Nanoengineering, Graduate School of Science & Engineering, Waseda University

## April 2004 - March 2007

Dr.Eng., Department of Nanoscience & Nanoengineering, Graduate School of Science & Engineering, Waseda University

# **Working History:**

# April 2004 - March 2006

21COE Research Assistant, 21COE 'Practical Nanochemistry', Waseda University

# April 2006 - March 2007

Research Fellowship for Young Scientists from the Japan Society for the Promotion of Science (JSPS)

# **April 2007 - Sep. 2007**

Researcher (Tenure), International Center for Young Scientists (ICYS), NIMS

#### Oct. 2007 - March 2016

Independent Scientist (Tenure), MANA, NIMS

# April 2016 - May 2016

Group Leader & MANA-PI (Tenure), MANA, NIMS

# May 2016 - Nov. 2017

Professor (Tenure), Australian Institute for Innovative Materials (AIIM), University of Wollongong

## Nov. 2017 - Present

Professor (Tenure), School of Chemical Engineering, The University of Queensland

#### Nov. 2017 - Present

Senior Group Leader, Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland

#### Awards:

2007 Mizuno Award by Department of Applied Chemistry, Waseda University

2010 The Ceramic Society of Japan (CerSJ) Award for Advancements in Ceramic Science and Technology

- 2010 Inoue Research Award for Young Scientists
- 2012 PCCP Prize by the Royal Society of Chemistry (RSC)
- 2012 The Tsukuba Encouragement Prize
- 2013 The Young Scientists' Prize by the Ministry of Education, Culture, Sports, Science and Technology (MEXT)
- 2014 The Best Paper Prize, Science and Technology of Advanced Materials (STAM)
- 2014 The Chemical Society of Japan (CSJ) Award for Young Chemists
- 2016 The Most Cited Researchers: Developed for ShanghaiRanking's Global Ranking of Academic Subjects 2016 by Elsevier (Chemical Eng.)
- 2016 Thomson Reuters' Highly Cited Researchers 2016 (Chemistry)



2016 NISTEP Award (National Institute of Science and Technology Policy, Japan)

- 2017 Thomson Reuters' Highly Cited Researchers 2017 (Chemistry)
- 2018 Thomson Reuters' Highly Cited Researchers 2017 (Chemistry)

#### **Honors:**

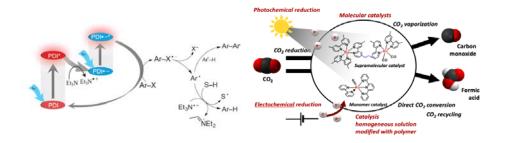
- 2008-Present Visiting Professor, Waseda University, Japan
- 2008-2015 PRESTO Researcher, Japan Science and Technology Agency (JST)
- 2011-Present Visiting Professor, Tianjin University, China
- 2013-2016 Visiting Professor, University of Wollongong, Australia
- 2013-2017 Associate Editor, APL Materials, The American Institute of Physics (AIP)
- 2014-Present Editorial Board Member, Scientific Reports, Nature Publishing Group (NPG)
- 2014-Present Editorial Board Member, Turkish Journal of Chemistry
- 2014-Present Editorial Board Member, Journal of Inorganic and Organometallic Polymers and Materials
- 2015-Present Visiting Professor, King Saud University, Saudi Arabia
- 2016-Present Review Editor, Science and Technology of Advanced Materials (STAM)
- 2016 Present Hortatory Group Leader & MANA-PI, Mesoscale Materials Chemistry Group, MANA, NIMS
- 2017-Present Visiting Professor, NanJing Tech University, China

# Photocatalysis Mechanisms and Polymer Chromophore-Catalyst Assemblies

#### Kirk S. Schanze

Department of Chemistry, University of Texas at San Antonio, San Antonio, TX 78249 Email: kirk.schanze@utsa.edu

The talk will highlight recent mechanistic work that has explored the mechanism of photocatalysis by organic perylene diimide anion radicals as well as photocatalysis with polymer chromophore catalyst assemblies. In the first segment, research will be highlighted that is related to the use of perylene diimide dyes as photocatalysts for reductive reactions of organic substrates. In particular, previous work<sup>1</sup> suggests that the excited state of the perylene diimide anion radical can act as a powerful photoreductant to catalyze dehalogenation reactions of aryl halides (ArX). By using picosecond transient absorption spectroscopy, we have directly observed the photoinduced electron transfer reaction between the doublet excited state of the perylene diimide anion radical (\*Per<sup>-</sup>) and ArX. Further, find that this excited state is able to reduce ArX with reduction potentials less negative than -1.6 V. Importantly, \*Per<sup>-</sup> does not appear to be able to reduce ArX with more negative reduction potentials. This latter observation conflicts with previous mechanistic conclusions. A second line of work that will be explored concerns our recent development of polystyrene-based chromophore-catalyst assemblies that can be used for CO<sub>2</sub> reduction.



#### References

Ghosh, I.; Ghosh, T.; Bardagi, J. I.; König, B. Reduction of Aryl Halides by Consecutive Visible Light-Induced Electron Transfer Processes, *Science* **2014**, *346*, 725-728

# Prof. Kirk S. Schanze

**Bio-sketch:**Kirk Schanze earned his B.S. in Chemistry from Florida State University in 1979 and his Ph.D. in Chemistry from the University of North Carolina at Chapel Hill in 1983. He was appointed a Miller Postdoctoral Fellow at the University of California, Berkeley, from 1984-1986 and began his independent faculty career at the University of Florida in 1986. Schanze was University Distinguished Professor and Prominski Professor of Chemistry at the University of Florida until 2016. He is currently the Robert A. Welch



Distinguished University Professor at the University of Texas at San Antonio. He was a Senior Editor of the ACS journal *Langmuir* from 2000 - 2008. Since 2008, Schanze is Editor-in-Chief of *ACS Applied Materials & Interfaces*, the ACS journal focused on chemistry and engineering of applications-focused research in materials and interfaces.

Schanze's research is focused on the field of light-matter interactions in molecular, polymer and materials systems. His group has developed and studied materials with applications in luminescence, chemo- and bio-sensing, light emitting diodes, solar cells and solar fuels. He has authored or co-authored 300 peer-reviewed articles on basic and applied research topics, with a primary focus on organic and organometallic materials chemistry, and is named in 20 patents or disclosures.

# Green Chemistry by Nanoporous Catalysts Microwave Synthesis,

# **Organofunctionality & Hierarchy**

# Prof. Sang-Eon Park (朴尙彦)

Department of Chemistry
Inha University, Incheon 22212, South Korea. <a href="mailto:separk@inha.ac.kr">separk@inha.ac.kr</a>

Green chemistry approaches have become crucial not only in the chemistry but also in the environment & energy sector in order to achieve sustainability in the future. And among many of approaches and principles for green engineering as well as green chemistry, the role of catalysis is very pivotal to reach the goals for atom efficiency, reduction in waste, energy saving and etc..

Nanoporous materials such as mesoporous materials and zeolites have been powerful as heterogeneous catalysts by providing the confined space to improve catalysis but have some challenges for environmental-friendly synthesis, coke resistance, and larger molecule reactions due to molecular dimension pores, which require the hierarchical topology having both meso- and micro-pores.

Zeolites and some nanoporous materials have been synthesized by microwave, which gave shortened synthesis times for energy saving as well as some merits in topological syntheses that enable the controls on morphologies and pore structures as well as to have organofunctionality on the wall through in-situ synthesis, that allow organocatalysis.

The hierarchical zeolites where mesopores are co-existed with their intrinsic micropores within the zeolite crystals were considered to overcome the diffusional limitation as well as activity and selectivity improvement with coke stability for the catalytic reactions. Recently, great attention has been devoted to the development of meso-micro hierarchical zeolites but mostly far away from the commercial viable ways for applying to industry.

Here, several strategies for mesopore creation, such as soft and hard templating, process controlling and post-treating, have been proposed to prepare hierarchical zeolite materials by taking advantages of microwave synthesis to possess both mesoporosity and microcrystallinity. Microwave syntheses for these hierarchical zeolites demonstrated to not only provide facile, fast, and economic way to synthesize but also superior controllability for mesopore generation.

And the role of mesoporosity generated by microwave synthesis was demonstrated in the catalytic reactions of relatively bulky molecules.

# **Prof. Sang-Eon Park**

Lab. of Nano-Green Catalysis and Nano Center for Fine Chemicals Fusion Technology, Dep't of Chemistry & Chem. Engineering, Inha University, Incheon 402-751, Korea, E-mail: <a href="mailto:separk@inha.ac.kr">separk@inha.ac.kr</a>

#### **Education**

1975 B.S. Applied Chem., College of Eng., SNU 1977 M.S. Chemistry, KAIST 1981 PhD. Chemistry, KAIST

# **Experience**

1984-1986 Post-Doc; Taxas A&M Univ., USA
1975-1984 Research Scientist, Chon Eng. Co.
1987-2003 Chem. Tech. Division, KRICT
2003-Present Prof. in Chemistry, Inha Univ.
2004-Present Director of Nano Center, Inha Univ.
2005-2014 IFP(Inha Fellowship Professor)
2012-2014 HaeCheon Prof. in Dalian Tech. Univ.
2009-2014 Outside Director of S-Oil
2017~ FRSC (Fellow of Royal Society of Chemistry)



#### **Activities**

- Journal of CO2 Utilization (Elsevier, Oxford); Editor-in-Chief
- Journal of Advanced Porous materials; International Advisory Board Member
- •Green Chemistry Journal (RSC); International Advisory Board Member
- •International Advisory Board and Scientific Committee Members : ICCDU, ZMPC18, IMMS
- •Bulletin of the Catalysis Society of India, Editorial Board Members

Korean Representative of AON Green Chemistry

Euro-Asia Journal of Applied Science (Editorial Board)

ACS, Petroleum Division (Executive Committee Member)

Associative Editor: Bull. Korean. Chem. Soc.

Research on Chemical Intermediates (Editorial Board)

Inorganic Chemistry Division Head: KCS

Catalysis Division Chairman: KIChE

Scientific Committee Member of 14th ICC

7th International Conference on Carbon dioxide Utilization (2003, Secretary)

2nd IMMS Co-Chairman

Inter. Advisory member of the 1st International Conference on Green & Sustainable Chemistry 11th IZC Pre-chool Co-Chairman

# **Invited lectures**

# (Plenary lectures)

- •CatSymp 23(2018) Plenary Bengalore, India
- •IMMS- Challenges and Strategies in Catalysis by Organic-Inorganic Hybrid Mesoporous Materials (2013)
- •ICCDU-2013, 2009 O<sub>2</sub> Activation for the Use as Oxidant (2013)
- •JKSC14 -Catalytic activation of CO<sub>2</sub> as soft oxidant and promoter (2013) (Key-note Lectures)
- •PMRD 2018, 2017- Ket Note Lecture, Cairo
- 8th World Congress on Oxidation Catalysis 2017
- ACS 2008, 2012, 2013
- ICCDU 2015; ICCDU 2016; ICCDU 2017 : Role of CO<sub>2</sub> in the oxidative conversions

# Awards:

2001 KCS Technical Axhievement Award

2003 KCS Scientific Achievement Award

2001 ACS Best Paper Awatd

2002 ACS Best Presentation Award

2005 Angewante Chemie VIP Paper (Willey)

2006 KSIEC Award (KSIEC)

2007 Best Scientist Award of IncheonCity

2008 YeoSanCatalysis Award (KIChE)

2017 FRSC (Fellow of Royal Society of Chemistry)

#### **Publication:**

450 Scientific papers, 75 Patents; Commercialization: 6

1) H<sub>2</sub>-PSA, 2) Alkylation, 3) Zeolite MW Synthesis,

4) H<sub>2</sub>O<sub>2</sub> Process, 5) VOCs Catalyst 6) Reformer

**Books** Edited (Nanomaterials in Korean;

Stud. in Surf. Sci.: Vol. 102, 146, & 153.

Book Chapters: 12

# Research Areas:

CO<sub>2</sub> and CH<sub>4</sub> Chemistry

Green Oxidation CO<sub>2</sub> as promoter

Activation of CO<sub>2</sub> as Soft Oxidant

Green Chemistry via Nanocatalysis Morphosynthesis of NanoporousMat' ls by Microwave

Nano assembly of zeolitic materials Para-xylene maximizing

Solid-state Supramolecular Synthesis Energy and Environmental Alleviation by Nanocatalyst Acid-Base Catalysis

# Supramolecular Photocatalyts for Pollutant Degradation and Tumor

# Removal

Yongfa Zhu

Department of Chemistry, Tsinghua University, Beijing, China zhuyf@tsinghua.edu.cn

A new class of organic supramolecular photocatalysts with full visible spectrum response has been successfully developed. The texture structure, crystal structure, photoelectric physicochemical properties, organic electron energy band structure, photocatalytic oxidation and anticancer properties can be adjusted via molecular structure and stacking structure. The degradation ability, water splitting ability and anticancer came from the HOMO and LUMO level. The photocatalytic activity came from molecular dipole, ordered stacking and nanostructure.

Self-assembled PDINH supramolecular is an effective visible-light photocatalyst for the photodegradation of pollutants and even split water for oxygen evolution. Compared with monomeric PDINH, self-assembled PDINH supramolecular have band-like electronic energy level structure similar to inorganic semiconductor due to orbital overlaps between PDINH-molecular units. Strong  $\pi$ - $\pi$  stacking between PDINH molecules enables effective long-range electrons delocalization and accordingly promotes photo-generated charge migration and separation, leading to its remarkable photocatalytic activity.

Supramolecular organic nanofibers, self-assembled by a carboxy-substituent PDI molecule via H-type  $\pi$ - $\pi$  stacking and hydrogen bonding, can act as an effective photocatalyst for both organic pollutants degradation and water oxidation under full visible light. The high activity came from the molecular dipole and the nanocrystallization. Higher  $\pi$ - $\pi$  supramolecular packing leads to a smaller bandgap, a deeper valence band position, enhanced light absorption and photo-oxidation capability. The inter-electronic field raised from ordered dipole can effectively promote the migration and separation of photo-generated carriers. H/J-type aggregated PDI supramolecular nanostructures were constructed via length of linear carboxysubstituent side-chains. H-aggregates have higher  $\pi$ -electron conjugation and show more semiconductor characteristics, which results in higher carrier separation and migration efficiency. Whereas, J-aggregates exhibit more molecular properties due to low  $\pi$ -electron conjugation caused by head-to-tail stacking mode. H-aggregated PDI mainly forms superoxide radicals (·O<sup>2</sup>-) and holes (h+) through electron-transfer (ET). In contrast, Jaggregated PDI mainly generates singlet oxygen species (<sup>1</sup>O<sub>2</sub>) via energy-transfer (EnT). Benefit from the stronger oxidization ability of O<sup>2</sup>- and h<sup>+</sup>, H-aggregated PDI shows higher photocatalytic activity for degradation and oxygen evolution under visible light. Whereas, Jaggregated PDI exhibits good photocatalytic anti-cancer activity owing to short length of nanofiber.

The full spectrum responsive supramolecular photocatalyst, SA-TCPP has been synthesized via an easy-conducted  $\pi$ - $\pi$  stacking. The SA-TCPP can powerfully spilt water to hydrogen

and oxygen at 40.8 and 36.1  $\mu$ mol·g-1·h-1 without co-catalyst. The organic pollutants can be efficiently mineralized by the SA-TCPP under visible light irradiation. The degradation performances of SA-TCPP were over 10 times better than the inorganic photocatalysts. The single crystalline structure of  $\pi$ - $\pi$  stacking promoted the transportation and separation of photogenerated carriers. Supramolecular photocatalyst SA-TCCP of bio-safe amount, targeted injection into the solid tumor inside, completely kill the tumor within 10 min under the deep penetration of red light (600-700 nm) irradiation. Photogenerated holes work as the most significant radical in the photocatalytic therapy process, which is abundant on the surface of photocatalyst in cytoplasm. The solid tumors was completely removed via photocatalysts injection and red-light irradiation.

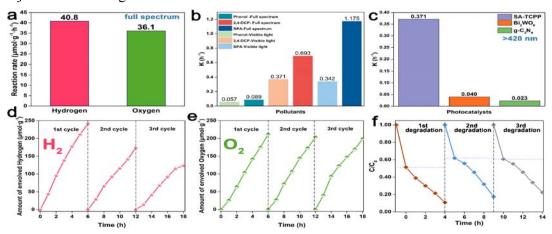


Fig. 1. Photocatalytic water splitting and degradation of pollutants. (a) Photocatalytic water splitting reaction rate of SA-TCPP under full spectrum; (b) Apparent rate constants k of degradation reactions for different pollutants under visible light and full spectrum; (c)Comparison of apparent rate constants k of different photocatalysts for 5.00 ppm 2,4-DCP degradation; (d) Cyclic reactions of hydrogen evolution with trolamine as hole scavenger; (e) Cyclic reactions of oxygen evolution with AgNO3 as electrons scavenger; (f) Cyclic degradations of 5.00 ppm 2,4-DCP.

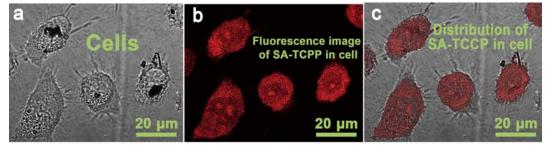


Figure 2.The distribution of SA-TCPP in cancer cells. (a) Bright-field image and (b) Fluorescence image of Hela cells incubated with SA-TCPP, (c) overlap of (a) and (b).

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# Prof. Yongfa Zhu

Dr. Yongfa Zhu received his BA degree in 1985 from Nanjing University and obtained his master degree in 1988 from Peking University. He had studied and worked at Tsinghua University since 1992 to now and received a PhD degree at 1995. He is currently a full professor of Tsinghua University and associate editor for *Applied Catalysis B*.

His current research is focused on photocatalysis and application on environmental, energy conversion and anti-tumor. He is the author and co-author of 329 original research papers published in SCI journals. The total cited numbers reached about 22800 and the H-index arrived at 81. About 34 papers was selected as High-Cited Papers by Essential Science Indicators. Besides, he has written about 5 books and applied about 24 patents.

	<b>Education:</b>			
	1981-1985	Nanjing	University	Chemistry
	B.Sc.			
	1985-1988	B Pekin University Chemistry		
	M.Sc.			
	1992-1995	Tsinghua Un	iversity Chemis	try Ph.D.
	Academic and Professional Experience:			
	1988-1992 Assistant Professor, Tsinghua University			
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# The Physics of Contact-Electrification and Its Implication to New

# **Energy Science**

**Zhong Lin Wang** 

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LISA

Contact electrification (triboelectrification) effect, the most fundamental effect for electricity, has been known for over 2600 years since ancient Greek time, but its scientific mechanism remains unclear. The study of triboelectrification is recently revived due to the invention of the triboelectric nanogenerators (TENGs) by using the coupling of triboelectrification and electrostatic induction effects, which is the most effective approach for converting tiny mechanical energy into electricity for powering small sensors. TENG is playing a vitally important role in the distributed energy and self-powered systems, with applications in internet of things, environmental/infrastructural monitoring, medical science, environmental science and security. In this talk, we first present the physical mechanism of triboelectrification for general materials. The charge transfers between a case such as a metaldielectric was attributed to the electron transfer between the filled states up to the Fermi level as governed by the Fermi-Dirac function. For the case of dielectric-dielectric, the charge transfer was attributed to between the surface states of the two materials. For a general case that the system cannot be described by a state surface model, an electron cloud-potential well model is proposed based on the overlap of electron wave functions across two atoms, which can be generally applied to explain all types of CE in conventional materials. Secondly, the fundamental theory of the TENGs is explored based on the Maxwell equations. In the Maxwell's displacement current proposed in 1861, the term E/t gives the birth of electromagnetic wave, which is the foundation of wireless communication, radar and later the information technology. Our study indicates that, owing to the presence of surface polarization charges present on the surfaces of the dielectric media in TENG, an additional term  $P_{s}/t$  should be added in the Maxwell's displacement current, which is the output electric current of the TENG. Therefore, our TENGs are the applications of Maxwell's displacement current in energy and sensors. TENGs have three major application fields: micro/nano-power source, self-powered sensors and blue energy. We will present the applications of the TENGs for harvesting all kind mechanical energy that is available but wasted in our daily life, such as human motion, walking, vibration, mechanical triggering, rotating tire, wind, flowing water and more. Then, we will illustrate the networks based on triboelectric TENGs for harvesting ocean water wave energy, for exploring its possibility as a sustainable large-scale blue energy. Lastly, we will show that TENGs as self-powered sensors for actively detecting the static and dynamic processes arising from mechanical agitation using the voltage and current output signals.

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- Z.L. Wang, J. Chen, L. Lin "Progress in triboelectric nanogenertors as new energy technology and self-powered sensors", Energy & Environmental Sci, 8 (2015) 2250-2282.

# **Prof. Zhonglin Wang**

Dr. Zhong Lin (ZL) Wang received his PhD from Arizona State University in 1987. He is the Hightower Chair in Materials Science and Engineering and Regents' Professor at Georgia Tech.

Dr. Wang is a pioneer and world leader in nanoscience and nanotechnology for his outstanding creativity and productivity. He has authored and co-authored 6 scientific textbooks and over **1200** peer reviewed reference and journal articles (40 in Nature, Science and their family journals), 45 review papers and book chapters, edited and co-edited 14 volumes of books on nanotechnology, and held over 100 US and foreign patents. Dr. Wang is the world's top 5 most cited authors in nanotechnology. From SCI data base, his entire publications have been cited for over 114,000 times with an h-index of 166 [ResearcherID]. Google scholar gives a citation of 156,000 with an h-index of 196 [Google Scholars]. He has delivered over 900 plenaries, keynotes, invited and seminar talks at international and national conferences as well as universities and research institutes worldwide.

Eni Award in Energy Frontiers (2018); American Chemical Soc. Publication most prolific author; Global Nanoenergy Prize, The NANOSMAT Society, UK (2017); Distinguished Research Award, Pan Wen Yuan foundation (2017); European Advanced Materials Laureate (2016); Outstanding Achievement in Research Innovation award, Georgia Tech (2016); Distinguished Scientist Award from (US) Southeastern Universities Research Association (2016); Thomas Router Citation Laureate in Physics (2015); World Technology Award (Materials) (2014); Distinguished Professor Award (Highest faculty honor at Georgia Tech) (2014); NANOSMAT prize (United Kingdom) (2014); China International Science and Technology Collaboration Award, China, (2014); The James C. McGroddy Prize in New Materials from American Physical Society (2014); ACS Nano Lectureship (2013); Edward Orton Memorial Lecture Award, American Ceramic Society (2012); MRS Medal from Materials Research Soci. (2011); Dow Lecture, Northwestern University (2011); Hubei Province Bianzhong award (2009); Purdy award, American Ceramic Society (2009); John M. Cowley Distinguished Lecture, Arizona State University (2012); Lee Hsun Lecture Award, Institute of Metal Research, China (2006); NanoTech Briefs, Top50 award (2005); Sigma Xi sustain research awards, Georgia Tech (2005); Georgia Tech faculty outstanding research author award (2004); S.T. Li Prize for Distinguished Achievement in Science and Technology (2001); Outstanding Research Author Award, Georgia Tech (2000); Burton Medal, Microscopy Soc. of America (1999); Outstanding Oversea Young Scientists award from NSF China (1998); NSF CAREER (1998).

Dr. Wang was elected as a foreign member of the Chinese Academy of Sciences in 2009, member of European Academy of Sciences in 2002, fellow of American Physical Society in 2005, fellow of AAAS in 2006, fellow of Materials Research Society in 2008, fellow of Microscopy Society of America in 2010, fellow of the World Innovation Foundation in 2002, fellow of Royal Society of Chemistry, and fellow of World Technology Network 2014. He is an honorable professor of over 10 universities in China and Europe.

Dr. Wang is the founding editor and chief editor of an international journal *Nano Energy*, which now has an impact factor of 11.55.

Dr. Wang's breakthrough researches in the last 15 years have been featured by over 50 media world wide including CNN, BBC, FOX News, New York Times, Washington Post, Reuters, NPR radio, Time Magazine, National Geography Magazine, Discovery Magazine, New Scientists, and Scientific America.

Dr. Wang is the #25 in the list of **the world's greatest scientists**.

# Semiconductor Nanomaterials for Photoelectrochemcial

# **Water Splitting**

# Lianzhou Wang

Nanomaterials Centre, School of Chemical Engineering and Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St Lucia, 4072, QLD Australia (Email: l.wang@uq.edu.au)

Semiconducting materials hold the key for efficient photocatalytic and photoelectrochemical water splitting. In this talk, we will give a brief overview of our recent progresses in designing semiconductor metal oxides materials for photoelectrochemical energy conversion including photocatalytic solar fuel generation. In more details, we have been focusing the following a few aspects; 1) band-gap engineering of layered semiconductor compounds including layered titanate, tantalate and niobate-based metal oxide compounds for visible light phtocatalysis, and 2) two-dimensional nanosheets/nanoplates of TiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, WO<sub>3</sub>, BiVO<sub>4</sub> as building blocks for new photoelectrode design, and 3) the combination of a high performance photoelectrode BiVO<sub>4</sub> with perovskite solar cells can lead to unassisted solar driven water splitting process with solar-to-hydrogen conversion efficiency of >6.5%. The resultant material systems exhibited efficient visible light photocatalytic performance and improved power conversion efficiency in solar energy, which underpin important solar-energy conversion applications including solar fuel generation.

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- 5. Angew. Chem, 2019, doi/10.1002/anie.201810583
- 6. Chem. Rev., 2019, DOI: 10.1021/acs.chemrev.8b00584

# **Prof. Lianzhou Wang**

# **Biography:**

Lianzhou Wang is currently Professor in School of Chemical Engineering, Director of Nanomaterials Centre (Nanomac), and Senior Group Leader of Australian Institute for Bioengineering and Nanotechnology, the University of Queensland. He received his PhD degree from Shanghai Institute of Ceramics, Chinese Academy of Sciences in 1999. Before joining UQ in 2004, he has worked at two leading national research institutions (NIMS and AIST) of Japan as a research fellow for five years. Since joining UQ, he has worked/working as ARC Queen Elizabeth II Fellow (2006), Senior Lecturer (2007), Associate Professor (2010), and Professor (2012-) in School of Chemical Engineering and Nanomac.

#### Research:

Professor Wang's research focuses on the synthesis, characterisation and application of semiconductor nanomaterials for use in renewable energy conversion/storage systems including photocatalytsts for solar hydrogen and valuable chemical production, rechargeable batteries and low cost solar cells. In late 2018, his team has broken the certified efficiency world record of quantum dot solar cells, achieving 16.6%, which was recognised in the highly influential **Best** Research-Cell Efficiencies chart (https://en.wikipedia.org/wiki/Solar cell efficiency). In the last ten years' time, as a Chief Investigator, he has succeeded in winning 23 competitive ARC grants, two CSIRO Flagship Cluster projects, two CRC programs, and a number of industry funds. Prof. Wang has contributed 3 edited books, 12 edited book chapters, more than 330 journal publications (including top ranking journals such as Chem. Rev., Chem Soc. Rev., Angew. Chem., Adv. Mater., J. Am Chem. Soc., etc.), 12 patents and delivered over 100 plenary/keynote/invited presentations. He is serving as Associate Editor of Journal of Nanoparticles Research and Science Bulletin and is also on the Editorial Boards of other 3 international journals. He also won some prestigious Fellowships/awards including STA Fellowship of Japan, ARC QEII Fellowship, UQ Research Excellence Award of 2008, Scopus Young Researcher Award of 2011 (Engineering and Technology category), and ARC Future Fellowship of 2012, and is the fellow of Royal Society of Chemistry.

# **Current Projects**

- ARC Discovery Project, 2019-2021: <u>A New Photoelectrochemical System for Solar Hydrogen and Electricity</u>
- ARC Linkage Project: 2018-2021, New High Energy Density Cathode Materials for Lithium Ion Batteries
- ARC Discovery Project: 2017-2019, Perovskite Materials: exploring new properties beyond solar cells,
- CRC-P Project: 2017-2020, Printed Batteries
- ARC Linkage Project: 2016-2019, Design of New Two-dimensional Materials for

# Lithium Sulfur Batteries,

- Baosteel Australian-China Joint Research grant: 2016-2019, , new cathode materials for high performance Li-ion batteries,
- ARC DP, 2016-2018: Bifunctional Photocatalytic System for Water treatment and hydrogen production,
- ARC LIEF, 2016: Time-resolved terahertz and optical spectroscopy facility,
- ARC Linkage Project, 2015-2017, Understanding the role of nanoparticles in water based lubrication,
- ARC Future Fellowship (2012-2016): Designing new layered materials for efficient solar energy conversion
- CRC Polymer program (2012-2017): New barrier materials for solar cells

# **Investigating Environmental Catalysis using the Tools of Surface**

# **Science**

Steven L. Bernasek

Professor of Science, Yale-NUS College Singapore Professor of Chemistry-Emeritus, Princeton University

The tools of surface science, including photoelectron spectroscopy, electron diffraction, and scanning tunneling and atomic force microscopy, have provided and continue to provide important information about the mechanisms of heterogeneous catalytic reactions, particularly in catalytic systems of environmental importance. In addition to tools of this type, the emphasis on the use of well characterized model systems to examine reaction mechanisms in heterogeneous catalysis, has also contributed to our deepening understanding of these important and complex chemical processes. Examples will be presented of this combination of tools and model systems applied specifically to important problems of environmental heterogeneous catalysis.

The dry reforming of methane with CO<sub>2</sub> is a process that converts two major greenhouse gases into synthesis gas (CO + H<sub>2</sub>). Studies combining near-ambient pressure XPS, low energy electron diffraction, and scanning tunneling microscopy to investigate this reaction on the Ni(111) surface identify the presence of dynamic Ni-O phases. These O species appear to optimize CH<sub>4</sub> activation while improving coking resistance1. NAP-XPS studies of Pt nanoparticles supported on alumina in commercial catalysts used as diesel oxidation catalysts show an increase in Pt oxidation state especially in the presence of NO and O<sub>2</sub> under reaction conditions modelling exhaust composition2. NAP-XPS, UPS, and LEED studies of CO<sub>2</sub> hydrogenation on the Cu(111) model surface show clear evidence of a formate intermediate which may be important for methanol synthesis on Cu catalysts3. Studies of Cu-zeolite catalysts using NAP-XPS and in-situ synchrotron based XAFS methods suggest mechanisms for Cu mobility and NO reduction in the presence of ammonia4 used in selective catalytic reduction and ammonia slip catalysts. In each of these cases, the combination of the tools of surface science and the use of well-characterized model systems has increased our mechanistic understanding of these complex processes.

This work was carried out in collaboration with researchers at Yale-NUS College, in the Department of Chemistry of the National University of Singapore, and in the Department of Chemical Engineering at the Royal Institute of Technology (KTH) in Stockholm. The work is supported by the Ministry of Education of Singapore.

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- 4 S.L. Bergman, S. Dahlin, L. Pettersson, and S.L. Bernasek, in preparation.

# Prof. Steven L. Bernasek

#### **Personal Information**

Birthdate: December 14, 1949 Birthplace: Holton, Kansas

Married: June 5, 1971 to Sandra Lynn Taylor

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Education

B.S. Chemistry, Magna cum Laude, Kansas State University, 1971

Ph.D. Chemistry, University of California, Berkeley, 1975.

# **Employment**

July 2015 to present Professor of Science, Yale-NUS College, Singapore

May 2017 to July 2018 Executive Vice President-Academic Affairs

Yale-NUS College, Singapore

July 2016 to May 2017 Dean of Faculty, Yale-NUS College, Singapore

July 2015 to July 2016 Director Division of Science

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July 2015 to present Professor of Chemistry Emeritus, Princeton University

July 1986 to July 2015 Professor of Chemistry, Princeton University

Sept 2014 to Feb 2015 Interim Division Director

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Jan. 2004 to July 2004 Acting Chairman, Chemistry, Princeton University

S.L. Bernasek, Page 2

July 1996 to July 2004 Associate Chairman, Chemistry, Princeton University

Sept 1992 to Sept. 2007 Off Site, Part Time Program Officer

Chemistry Division, National Science Foundation

Sept 1991-August 1992 Visiting Scientist, Chemistry Division

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July 1981 to June 1986 Associate Professor of Chemistry

July 1975 to June 1981 Assistant Professor of Chemistry

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## **Honors and Awards**

- Putnam Scholar, Kansas State University, 1967-1971
- H.H. King Chemistry Scholarship, Kansas State University, 1967-1971
- Phi Eta Sigma
- Phi Kappa Phi
- National Science Foundation Graduate Fellow, 1971-1975
- Woodrow Wilson Fellowship Finalist, 1971
- DuPont Young Faculty Grant, 1977
- ACS-Exxon Award in Solid State Chemistry, 1981
- Alexander von Humboldt Foundation Research Fellow, 1985-1986, 1990, 2007

- Fellow of the American Association for the Advancement of Science, 1994
- Visiting Fellow, JILA, University of Colorado, 1999
- Distinguished Visiting Professor, National University of Singapore, 1998, 2000, 2003, 2007,

2010, 2011, 2012, 2014

- Moses Gomberg Lecturer, University of Michigan, 2001
- Fellow of the American Vacuum Society, 2001
- ACS Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry, 2006
- -ACS Petroleum Research Fund Advisory Board, 2009-2015
- -KOSMOS Fellow, Humboldt University-Berlin, 2014-2015
- -King Faisal Prize in Science, Award Committee, 2019

# **Solid-State-NMR Characterization of functional Materials**

# Gerd Buntkowsky

Institute of Physical Chemistry, Technical University Darmstadt, Alarich-Weiss-Str. 8, D-64287

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Recent results about standard and dynamic nuclear polarization (DNP) enhanced solid-state nuclear magnetic resonance (NMR) spectroscopy on nanostructured anf functional materials are reported. The first example reports studies on materials based on crystalline nanocellulose (CNC) or microcrystalline cellulose (MCC), which are used as support material for functionalization or in combination with heterocyclic molecules as ion conducting membranes. The second example reports studies on mixed metal oxides such as V-Mo-W oxides, which are employed as heterogeneous catalyst in bulk-scale production of basic chemicals. The third example reports solid-state NMR studies of lead-free perovskite materials, which are employed as environmentally benign substitution materials for conventional lead-based electronics materials. These materials are discussed in terms of their application and physico-chemical characterization by solid-state NMR techniques, combined with gas-phase NMR and quantum-chemical modelling on the density functional theory (DFT) level. Moreover, the analytic power of the combination of these techniques with DNP for the identification of low-concentrated carbon and nitrogen containing surface species in natural abundance is discussed.

# Prof. Gerd Buntkowsky



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**2. Research fields** Characterization of functional materials, heterogeneous catalysts, enzyme complexes and disordered systems by Solid-State NMR spectroscopy; Development and Application of Hyperpolarization Techniques (DNP, PHIP, SABRE) for signal enhancement of NMR and MRI; Spin-Dynamics and Reaction Kinetics.

## 3. Scientific career

- 1978 1982Study of Physics FU Berlin
- 1982 1986Diploma thesis in Physics, supervisor Hans-Martin Vieth
- 1983 1986Teaching assistant 70 h, Department of Physics, FU Berlin

1986 Diploma in Physics, Department of Physics, FU Berlin 1986 - 1990PhD thesis in Physics, supervisor Hans-Martin Vieth

1987 - 1991 Scientific co-worker, Department of Physics, FU Berlin

1991 PhD in Physics, Department of Physics, FU Berlin

1991 - 2004Senior researcher (Akad. Rat), Department of Chemistry, FU Berlin 2000 Habilitation in Physical Chemistry, Department of Chemistry, FU Berlin 2000 - 2010Private docent for Physical Chemistry, FU Berlin

2004 - 2009 Professor (C3) for Physical Chemistry, FSU Jena

2009 - Professor (W3, Chair) of Physical Chemistry, TU Darmstadt

# 4. Stipends & Awards

2011 Carlo and Karina Giersch Foundation Athene Special Award 2008 Offer W3 Professorship for Physical Chemistry, TU Darmstadt (accepted) 2004 Offer C3 Professorship for Physical Chemistry, FSU Jena (accepted) 1986 - 1987PhD Scholarship from the State of Berlin

# 5. Services to the community

Since 2010 Editorial board Solid State NMR Spectroscopy

2011 - 2017 Dean of the Faculty of Chemistry, TU Darmstadt

Since 2012 Elected member of the DFG Chemistry Review Board

2014 DAAD prime selection committee

Since 2016 Editorial board Applied Magnetic Resonance

Since 2016 Editorial board Zeitschrift für Physikalische Chemie

# 6. Ten important publications from the last decade

- 1.) Total number (1989-2017) of peer-reviewed publications is 189
- 1. A. S. Kiryutin, G. Sauer, A. V. Yurkovskaya, H.-H. Limbach, K. L. Ivanov\*, G. Buntkowsky\*, Parahydrogen allows Ultra-sensitive indirect NMR Detection of Catalytic Hydrogen Complexes, J.Phys.Chem. C., (2017), 121, 9879-9888
- 2. M. M. Hoffmann\*, S. Bothe, T. Gutmann\*, F. Hartmann, M. Reggelin, G. Buntkowsky\*, Directly vs. Indirectly enhanced <sup>13</sup>C in Dynamic Nuclear Polarization Magic Angle Spinning NMR Experiments of Nonionic Surfactant Systems, J.Phys.Chem. C, (2017), 121, 2418–2427.
- 3. P. B. Groszewicz, M. Gröting, H. Breitzke, W. Jo, K. Albe, G. Buntkowsky\*, J. Rödel\*, Reconciling Local Structure Disorder and the Relaxor State in (Bi<sub>1/2</sub>Na<sub>1/2</sub>)TiO<sub>3</sub>-BaTiO<sub>3</sub>, Scientific Reports, (2016), 6, 31739.
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- 6. A. Tietze, D. Tietze, O. Ohlenschläger, E. Leipold, F. Ullrich, T. Kühl, A. Mischo, G. Buntkowsky, M. Görlach, S. H. Heinemann, D. Imhof, Structurally diverse µ-conotoxin PIIIA isomers block sodium channel NaV1.4, Angewandte Chemie Int.Ed., (2012), 51, 4058-4061
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- 8. D. Tietze, S. Voigt, D. Mollenhauer, M. Tischler, D. Imhof, T. Gutmann, L. González, O. Ohlenschläger, H. Breitzke, M. Görlach, <u>G. Buntkowsky\*</u>, "Revealing the position of the substrate in NiSOD: a model study", Angewandte Chemie Int.Ed., 50, (2011) 2946-2950
- 9. T. Gutmann, B. Walaszek, Y. Xu, M. Wächtler, I.de Rosal, A.Gruenberg, R. Poteau, R. Axet, G. Lavigne, B. Chaudret, H.-H. Limbach, <u>G. Buntkowsky\*</u>, Hydrido-ruthenium cluster complexes as models for reactive surface hydrogen species of ruthenium nanoparticles Solid-state <sup>2</sup>H NMR and quantum chemical calculations. J.Am.Chem.Soc., 132, (2010), 11759-11767
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# New Metal Alloy Electrocatalysts for the Reduction of CO<sub>2</sub> to

# **Multi-Carbon Products**

A. B. Bocarsly and A. R. Paris

# Princeton University

Binary alloys composed of a first row transition metal and either aluminum or gallium provide a new source of heterogeneous electrocatalysts for the reduction of CO<sub>2</sub> to both C1 products, and a variety of carbon-carbon bonded products. We have reported that Ni<sub>3</sub>Al reduces CO<sub>2</sub> to a variety of C3 oxygenates, <sup>1-2</sup> while Lewis et. al. has noted that various Ni<sub>x</sub>Ga<sub>y</sub> alloys generate C2 products from CO<sub>2</sub>. <sup>3</sup> In both cases, the higher order products are observed in low yield. However, these examples are important since they demonstrate that metallic systems that do not contain copper can form carbon-carbon bonds from CO<sub>2</sub>. Recently we discovered that appropriately selected bimetallic combinations can produce oxalate in high faradaic yields in aqueous electrolytes. In this case, a chromium-gallium system is found to give high yields of product.<sup>4</sup>

We are particularly interested in the Cr-Ga electrocatalyst since previous reports of oxalate electrogeneration from CO<sub>2</sub> necessitated the use of nonaqueous electrolytes. We find that CO<sub>2</sub> reduction can be carried out at potentials where oxalate formation competes favorably with H<sub>2</sub> production. Our new findings argue for a previously unexplored mechanism for the formation of carbon-carbon bonds that circumvents the generation of a [CO<sub>2</sub> intermediate. In addition, we find that this system is strongly solvent dependent, yielding a very large kinetic isotope effect when D<sub>2</sub>O is substituted for H<sub>2</sub>O in the electrolyte. A detailed mechanistic understanding of this type of system is likely to offer new opportunities for the electrosynthesis of multicarbon species with high faradaic yield and modest overpotential.

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- 2. Paris, A. R.; Bocarsly, A. B., "Mechanistic Insight into C2 and C3 Product Generation Using Ni<sub>3</sub>Al and Ni<sub>3</sub>Ga Electrocatalysts for CO<sub>2</sub> Reduction". In *Faraday Discussion on Artifical Photosynthesis*, Royal Society of Chemistry: Cambridge University, GB, **2018**.
- 3. Torelli, D. A.; Francis, S. A.; Crompton, J. C.; Javier, A.; Thompson, J. R.; Brunschwig, B. S.; Soriaga, M. P.; Lewis, N. S., "Nickel Gallium-Catalyzed Electrochemical Reduction of CO<sub>2</sub> to Highly Reduced Products at Low Overpotentials". *ACS Catalysis* **2016**,6 (3), 2100-2104.
- 4. Paris, A. R.; Bocarsly, A. B., "High-Efficiency Conversion of CO<sub>2</sub> to Oxalate in Water Is Possible Using a Cr-Ga Oxide Electrocatalyst". *ACS Catalysis* **2019**, 2324-2333.

### **Prof. Andrew Bocarsly**

Andrew Bocarsly received his Bachelor of Science degree jointly in chemistry and physics from UCLA in 1976, and his Ph.D. in chemistry from M.I.T. in 1980. He has been a member of the Princeton University, Chemistry Department faculty for thirty years. Professor Bocarsly has published over 175 <a href="majeres">papers</a> in peer reviewed journals and co-authored six patents. Research in his laboratory is focused on the materials chemistry associated with elevated temperature proton exchange membrane fuel cells, including composite membranes for elevated temperature cells and electrocatalysts for direct alcohol fuel cells; visible light photoelectrochemistry for the conversion of carbon dioxide to alcohols; cyanogel sol-gel processing routes to refractory materials, metal alloys and nanostructures; and molecule-based multielectron photoinduced charge transfer processes.

Professor Bocarsly serves as a consultant and contractor to various fuel cell and alternate energy companies. He is a founder and President of the Science Advisory Board for <u>Liquid Light Inc.</u>, a company formed to commercialize the formation of organic commodity chemicals from carbon dioxide using alternate energy sources. Professor Bocarsly has received an Alfred P. Sloan Fellowship, the Sigma Xi (Princeton Section) Science Educator Award, the American Chemical Society-Exxon Solid State Chemistry award, and serves as the electrochemistry editor for Methods in Materials Research. Presently, he is serving as a volume editor for Structure and Bonding in the area of fuel cells and batteries.

Thesis Advisor: Professor Mark S. Wrighton (currently, Chancellor, Washington University) Ph. D. Dissertation: "Characterization and Manipulation of Charge Transfer Processes at the Semiconductor Electrolyte Interface"

Professional Experience:

1994 - Present Professor of Chemistry, Princeton University

1987 – 1994 Associate Professor of Chemistry, Princeton University

1980 – 1987 Assistant Professor of Chemistry, Princeton University

1976 – 1980 Graduate Research Assistant, Massachusetts Institute of Technology

1975 Laboratory Assistant, Department of Chemistry, UCLA

1973 – 1974 Laboratory Assistant, Department of Chemical Engineering, UCLA University Activities:

1999 – present Academic Advisor, Mathey College

2002 – 2008 Committee of the Graduate School/Department of Chemistry DGS

2005 – 2006 Graduate School Subcommittee on Discipline

2006 – 2007 Graduate School Subcommittee on Policy

2007 – 2008 Graduate School Ad Hoc Subcommittee on Financial Policy

2007 – 2008 Graduate School Subcommittee on Curriculum

2008 McGraw Center University Internal Review Committee

2008 – 2009 Faculty Committee on Classrooms and Schedule

2011-2012 Council of the Princeton University Community

2011 I.P.Accelerator Fund Proposal Review Committee

2012 I.P.Accelerator Fund Proposal Review Committee

2013 – 2014 Faculty Committee on Classrooms and Schedule

2017 – 2019 Instrument Committee, Department of Chemistry

2017 - 2019 Graduate Studies Committee, Department of Chemistry

2016 – 2019 Organized Monthly Faculty Lunch Talks, Department of Chemistry

2016 - present PPPL, DOE Lithium Safety Site Committee

2016 – 2019 Chair, Imaging Center Committee (IAC), PRISM

2016 – 2019 PRISM Steering Committee

2017 – 2020 University Conflict of Interest Committee

2017 – 2020 University ESRM Committee

2018 – 2019 Faculty Committee on Classrooms and Schedule

Scholarly Symposia Organized:

2010 Host and organizer of an international workshop held in Frick on chemistry related to conversion of exhaust carbon dioxide to fuels.

2011 Organized and Chaired Symposium on CO2 activation chemistry in the Physical Chemistry

Division of the ACS for the Spring National Meeting, Anaheim, CA.

2012 Organized and Chaired the Second Biennial CO<sub>2</sub> Workshop, with operational support from Liquid Light Inc., the Princeton Department of Chemistry and Princeton's Andlinger Center. Held in Frick Laboratory.

2015 Organized and Chaired the Third Biennial CO<sub>2</sub> Workshop, with operational support from Liquid Light Inc., the Princeton Department of Chemistry. Held in Frick Laboratory.

2017 Co-organized a symposium on "Fundamental Aspects of Electrochemical Conversion of Carbon Dioxide" at the 232<sup>th</sup> National meeting of the Electrochemical Society.

2019 - 2022 Planning and hosting of ICCDU 2022 (International Conference on Carbon Dioxide Utilization)

Synergistic Activities:

Princeton Section ACS, Secretary-Treasurer (1992), Board Chair, (1994) and (2008)

Princeton Section ACS, Education Outreach and Executive Board Member (1992-)

Princeton University Quest, Elementary Science Teacher Training Program, Outreach Professor, (1996-2009)

Rider-Princeton CONNECT-ED, K-12 Science Teacher In Service Program, Advisory Board Member and Instructor (2001-2010)

Millennium Cell Inc., Science Advisor (New Jersey, 1995-2007)

New York - New Jersey Partners in Science Program, Director, (2000-2006)

Structure and Bonding, Editor, Volume 144 on Fuel Cells, (2007-2011)

Applied Semiconductor Inc., President of the Science Advisory Board (2008-2015)

Co-Founder, Liquid Light Inc. (2009-2017)

Liquid Light Inc., President of the Science Advisory Board (2009-2016)

Characterization of Materials, Assoc. Editor, Electrochemistry Section, (2000-2010)

Editorial Advisory Board Member, J. Physical Chemistry, (2013-2015)

Editorial Advisory Board Member, J. CO2 Utilization, (2017-present)

International Scientific Advisory Board, International Conference on Carbon Dioxide Utilization (2016-present)

Member of the Academic Committee of the Chinese Ministry International Joint laboratory on Resource Chemistry (2017-2022)

### Water Upgrading Chemistry Using Precious Metal Catalysis

Michael S. Wong<sup>1,2,3,4,5</sup>

Water is a natural resource that is fundamental to life on Earth, and providing access to clean water is one of the grand challenges in society. Population growth around the world not only exacerbates clean water sources for consumption, sanitation, household, and community needs, but also increases the water demand of agriculture and industry. As an enabling form of green chemistry, catalysis science can provide a new means to upgrade contaminated water to a quality level that matches its intended use, if operational constraints (ambient temperature, atmospheric pressure, variable water quality) can be overcome with materials with improved properties. Two example systems from my laboratory will be presented. Nitrate hydrogenation to dinitrogen using In-supported Pd will be discussed as a means to address the incomplete ability of ion-exchange adsorption methods to remove oxoanions from drinking water sources. Depending on the desired products (N2 versus NH3), I will show how the reaction selectivity can be controlled by reaction conditions and metal composition. The goldcatalyzed removal of organics from industrial wastewater (oil and gas produced waters) will be discussed also, using in situ hydrogen peroxide generated from air and organic hydrogen donors. I will explain how wastewater presents challenges to catalysis chemistry that, if surmounted, can provide opportunities for reuse of the treated water.

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<sup>&</sup>lt;sup>2</sup>Department of Chemistry

<sup>&</sup>lt;sup>3</sup>Department of Civil and Environmental Engineering

<sup>&</sup>lt;sup>4</sup>Department of Materials Science and NanoEngineering

<sup>&</sup>lt;sup>5</sup>Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment Rice University, Houston, TX, United States.

### Prof. Michael S. Wong

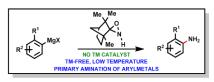
Dr. Michael S. Wong is Professor and Chair of the Department of Chemical and Biomolecular Engineering at Rice University. He was educated and trained at Caltech, MIT, and UC Santa Barbara. He is head of the Catalysis and Nanomaterials Laboratory (120+ publications, 20+ pending/issued patents, 300+ presentations, Google scholar h-index of 48, and ~10K+ citations, which tackles technical energy and sustainability issues through chemical engineering and materials chemistry approaches. He has received numerous honors over the years, including the MIT TR35 Young Innovator Award, the North American Catalysis Society/Southwest Catalysis Society Excellence in Applied Catalysis Award, and American Chemical Society Fellow.

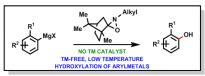
### **Practical & Environmentally Friendly Nitrogen-Transfer Processes**

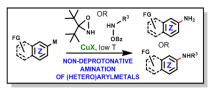
László Kürti, Ph.D., Associate Professor

Department of Chemistry, Rice University, Houston, TX 77030, USA

Amines and their derivatives are ubiquitous substances since they make up the overwhelming majority of drug molecules, agrochemicals as well as many compounds that are produced by plants and living organisms (i.e., natural products). Aromatic amines appear as substructures in more than one third of drug candidates. Not surprisingly, organic chemists spend a considerable amount of their time with the synthesis and late-stage functionalization of amines that serve as key chemical building blocks for the preparation of biologically active compounds, especially in medicinal chemistry. There is an urgent need for the development of novel carbon-nitrogen bond-forming methods and reagents that expand the toolbox of synthetic organic chemists and enable the environmentally friendly construction of complex molecular structures using the fewest number of chemical steps and generating the least amount waste.









Arylmetals are highly valuable carbon nucleophiles that are readily and inexpensively prepared either from aryl halides or directly from arenes and widely used on both laboratory and industrial scales to react with a wide range of electrophiles. Although C - C bond formation has been a staple of organic synthesis, the direct transfer of primary amino  $(-NH_2)$  and hydroxyl (-OH) groups to arylmetals in a scalable and environmentally friendly fashion remained a formidable synthetic challenge for decades because of the absence of suitable heteroatom-transfer reagents. The Kürti lab has demonstrated the use of bench-stable N - H and N - alkyl oxaziridines derived from readily available terpenoid scaffolds as efficient multifunctional reagents for the direct primary

amination and hydroxylation of structurally diverse aryl- and heteroarylmetals. This practical and scalable method provides one-step synthetic access to primary anilines and phenols at low temperature and avoids the use of transition-metal catalysts/ligands/additives, nitrogen-protecting groups, excess reagents and harsh workup conditions.

Subsequently, the Kürti group also developed the facile transfer of primary (-NH<sub>2</sub>) and secondary amino groups (-NHR) to heteroaryl- as well as arylcuprates at low temperature without the need for precious metal catalysts, ligands, excess reagents, protecting and/or

directing groups. This one-pot transformation allows unprecedented functional group tolerance and it is well-suited for the amination of electron-rich, electron-deficient as well as structurally complex (hetero)arylmetals. In some of the cases, only catalytic amounts of a copper(I) salt is required.

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- Zhou, Zhe; Ma, Zhiwei; Behnke, Nicole Erin; Gao, Hongyin and **Kürti, László**.\* "*Non-Deprotonative Primary and Secondary Amination of (Hetero)Arylmetals*." *J. Am. Chem. Soc.* **2017**, *139*, 115-118 (http://pubs.acs.org/doi/pdf/10.1021/jacs.6b12712).
- Padmanabha V. Kattamuri, Jun Yin, Surached Siriwongsup, Doo-Hyun Kwon, Daniel H. Ess\*, Qun Li, Guigen Li\*, Muhammed Yousufuddin, Paul F. Richardson, Scott C. Sutton and Kürti, László.\* "Practical Singly and Doubly Electrophilic Aminating Agents: A New, More Sustainable Platform for Carbon-Nitrogen Bond-Formation." J. Am. Chem. Soc. 2017, 139, 11184-11196. This article was featured in C&EN News: "Arymanines made easy", <a href="http://cen.acs.org/articles/95/i28/Arylamines-made-easy.html">http://cen.acs.org/articles/95/i28/Arylamines-made-easy.html</a> and Rice News: "Rice scientists simplify the incorporation of nitrogen into molecules", <a href="http://news.rice.edu/2017/07/12/rice-scientists-simplify-the-incorporation-of-nitrogen-into-molecules/">http://news.rice.edu/2017/07/12/rice-scientists-simplify-the-incorporation-of-nitrogen-into-molecules/</a>.

### Prof. László Kürti

### Associate Professor Department of Chemistry RICE UNIVERSITY

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Alternative E-mail: <u>kurti.laszlo@gmail.com</u> **EMPLOYMENT AND EDUCATION** 



•	Associate Professor - Tenure Track Position at Rice University,	<b>2015 June</b>
	Houston, TX	2010-2015
•	Assistant Professor - Tenure Track Position at UT Southwestern	
	Medical Center, Dallas, TX	
•	Postdoctoral Studies - Harvard University, Cambridge, MA	2006-2010
	(Professor Elias J. Corey)	
•	Ph.D. in Organic Chemistry - University of Pennsylvania,	2001-2006
	Philadelphia, PA (Prof. Amos B. Smith)	
•	Masters Degree in Organic Chemistry - University of Missouri,	<b>2001 June</b>
	Columbia, MO (Prof. M. Harmata)	
•	Diploma in Chemistry - University of Debrecen, Debrecen,	1998 June
	Hungary (Prof. Sándor Antus)	
•	<b>Diploma in English Hungarian Technical Translation</b> - University of Debrecen, Debrecen, Hungary	1997 June

### HONORS, AWARDS AND FELLOWSHIPS

- Biotage Young Principal Investigator Award November 2015
- NSF CAREER Award 2015-2020
- Japan Society for the Promotion of Science (JSPS) Fellowship August 2014 (Lecture tour in Japan in Nov 2014)
- Amgen Young Investigators' Award April 2014
- Thieme Chemistry Journal Award November 2010
- UTSWMC Endowed Scholar in Biomedical Research (startup funding) September 2010
- Best of Physical Sciences and Mathematics in Professional and Scholarly Publishing for Molecules and Medicine written by E.J. Corey, László Kürti and Barbara Czakó, 2008.
  - **Damon Runyon Cancer Fellowship** Awarded by the Damon Runyon Cancer Research Foundation June, **2007**
- Outstanding Academic Title designation by Choice Magazine for Strategic Applications of Named Reactions in Organic Synthesis written by László Kürti and Barbara Czakó.

#### TEXTBOOKS AND REFERENCE BOOKS

- Corey, E.J. and Kürti, LászlóEnantioselective Chemical Synthesis: Methods, Logic and Practice, Direct Book Publishing, LLC, Dallas, 2010. (Now owned, marketed & sold by ELSEVIER SCIENCE/Academic Press)
- Corey, E.J., Czakó, Barbara and Kürti, LászlóMolecules and Medicine, John Wiley and Sons Inc., New York, 2007.
- Kürti, LászlóandCzakó, Barbara Strategic Applications of Named Reactions in Organic Synthesis, Academic Press/Elsevier Science: Amsterdam 2005. Foreword by Professor E.J. Corey and Introduction by Professor K.C. Nicolaou.

### SELECTED RECENT PUBLICATIONS

- Ma, Zhiwei; Zhou, Zhe and Kürti, László.\* "Direct and Stereospecific Synthesis of N-H and N-Alkyl Aziridines from Unactivated Olefins Using Hydroxylamine O-Sulfonic Acids." Angew. Chem. Int. Ed. 2017, 56, 9986-9890. This article was featured in Rice News: "Greener molecular intermediates may drug design", <a href="http://news.rice.edu/2017/07/05/greener-molecular-intermediates-may-aid-drug-design/">http://news.rice.edu/2017/07/05/greener-molecular-intermediates-may-aid-drug-design/</a>.
- Jin-Zheng Wang, Jin Zhou, Chang Xu, Hongbin Sun\*, László Kürti\*, and Qing-Long Xu\*. "Symmetry in Cascade Chirality-Transfer Processes: A Catalytic Atroposelective Direct Arylation Approach to BINOL Derivatives." J. Am. Chem. Soc. 2016, 138, 5202-5205 (http://pubs.acs.org/doi/abs/10.1021/jacs.6b01458).
- Gao, Hongyin; Xu, Qing-Long; Keene, Craig; Yousufuddin, Muhammed; Ess, Daniel H.and **Kürti, László\***. "Practical Organocatalytic Synthesis of Functionalized Non-C<sub>2</sub>-Symmetrical Atropisomeric Biaryls." *Angew. Chem. Int. Ed.* **2016**, *55*, 566-571 (*Hot Paper*; <a href="http://onlinelibrary.wiley.com/doi/10.1002/anie.201508419/pdf">http://onlinelibrary.wiley.com/doi/10.1002/anie.201508419/pdf</a>).
- Gao, Hongyin; Xu, Qing-Long; Ess, Daniel H.and **Kürti, László\***. "Transition-Metal-Free, Low-Temperature Intramolecular Amination of Aromatic C-H Bonds: Rapid Synthesis of Fused Heterocycles." *Angew. Chem. Int. Ed.* **2014**, *53*, 2701-2705 (*Hot Paper*; http://onlinelibrary.wiley.com/doi/10.1002/anie.201309973/pdf).
- Xu, Qing-Long; Gao, Hongyin; Ess, Daniel H.and **Kürti, László\***. "Aerobic, Transition-Metal-Free, Direct and Regiospecific Mono-a-Arylation of Ketones: Synthetic Studies and Mechanism by DFT Calculations." *J. Am. Chem. Soc.* **2013**, *135*, 14048-14051 (<a href="http://pubs.acs.org/doi/pdf/10.1021/ja4074563">http://pubs.acs.org/doi/pdf/10.1021/ja4074563</a>).

### Furans as a Practical Chemical Resource for Oligosaccharides

George A. O'Doherty

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Oligosaccharides have long been recognized as an attractive renewable resource, as they are the major component of biomass. Because of the complex network that these carbohydrates monomers exist in, they are most frequently recovered as their dehydrated furan equivalents. Over the years the O' Doherty group has been working at the use of asymmetric catalysis for the practical synthesis of carbohydrate from simple achiral commodity chemicals, like furans. The success of this approach is evident by its ability to address a range of carbohydrate motifs, from monosaccharides to oligosaccharides. Fundamental to this approach is the development of highly efficient routes that transform, via catalysis, inexpensive achiral chemical resources (e.g., acylfuran 8) into enantiopure products (e.g., pyranone 2), which are poised for the conversion into complex carbohydrate motifs (e.g., oligomers 1, 3, 4). Recently, we have found that these approaches have matured to the point where we have developed enantioselective routes to these oligosaccharides in sufficient quantities that are amenable for biomedical investigations. An example of these types of approaches is outlined below (Scheme 1) in our recent approach to explore the anticancer activities of the cardiac glycoside oligosaccharides.

Scheme 1:Protecting group free de novo retrosynthetic approach to cardiac glycoside

### Prof. George A. O'Doherty

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#### **EDUCATION:**

The Ohio State University, Columbus, Ohio, Ph.D., Chemistry, Sept. 1987 to Jan. 1993,

Advisor: Professor Leo A. Paquette

Rensselaer Polytechnic Institute, Troy, New York, B.S., Chemistry, Sept. 1984 - June 1987

Advisor: Professor Alan R. Cutler

#### **SCIENTIFIC EMPLOYMENT:**

Full Professor Chemistry (Sept. 2010 - present): Department of Chemistry, Northeastern University

Full Member (2010): Mary Babb Randolph Cancer Center, West Virginia University

Associate Professor Chemistry (Aug. 2005 - Aug. 2010): Department of Chemistry, West Virginia University

Assistant Professor Chemistry (Sept. 2002 - Aug. 2005): Department of Chemistry, West Virginia University

### **HONORS and AWARDS:**

Horace S. Isbell Award from the ACS Carbohydrate Division (2009) Eberly College of Arts and Science Outstanding Researcher Award (2007) Woodburn Professor, Eberly College of Arts and Science (2006 & 2007) WVU's Dept. of Chemistry Outstanding Professor (2006)

Shanghai Normal University "Honored Professor" (Dec. 2005, 2010-2012)

Arnold and Mabel Beckman Young Investigator (Sept. 1999 to Aug. 2002)

NSF Postdoctoral Fellowship (Jan. 1993 to Dec. 1994)

British Petroleum America Fellowship (Jan. 1991 to Dec. 1991)

National Need Fellowship (Jan. 1989 to Dec. 1989)

OSU Departmental Fellowship (Sept. 1987 to Aug. 1988)

American Chemical Society (1987 to present)

American Society for Biochemistry and Molecular Biology (2012 to present) Visiting Professor at Indian Institute of Technology-Bombay (2015-2016)

**PUBLICATIONS (171):** This section is divided into four sections:

Research Articles (133), Reviews/Book Chapters (30), Book Reviews (3), and Patents (5)

### C-C Bond Formation Enabled by Radical Engaged Organocatalysis

Wei Wang<sup>a,b</sup>

<sup>a</sup> Department of Pharmacology and Toxicology, College of Pharmacy, BIO5 Institue and University of Arizona Cancer Cener, University of Arizona, Tucson, AZ 85721, USA; <sup>b</sup> School of Pharmacy, East China University of Science & Technology, Shanghai 200237, China E-mail: wwang@pharmacy.arizona.edu

C-C bond construction is the central goal in organic synthesis. Reecently, we initiated a program aiming at developing organocatalyzed radical engaged reactions for C-C bond formation. Toward this end, we have developed distinct C-C bond forming manifolds enabling incororation of various functionalities into readily accessible substances including aromatics, olefins, structurally complex natural products, peptides and sugars (Figure 1).<sup>1-7</sup>

$$R \nearrow X/H + -C - CO_2H \qquad \begin{array}{c} Organic Dye \\ Visible Light \\ \hline \\ O \end{array} \qquad + \qquad \begin{array}{c} HAT \ cat \\ (NH_4)_2S_2O_8 \\ \hline \\ O \end{array} \qquad \begin{array}{c} N \\ \hline \end{array}$$

Figure 1. Ogranocatalytic radical engaged C-C bond formation processes.

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- Liu, S.-H.; Liu, A.-Q.; Zhang, Y.-Q.; Wang, W. Chem. Sci., 2017, 8, 4044.
- Li, X.-M.; Huang, H.; Yu, C.-G.; Zhang, Y.-T.; Li, H.; Wang, W. Org. Lett., 2016, 18, 5744.

# Prof. Wei Wang



Dr. Wei Wang is Full Professor of Pharmacology & Toxicology and the director of drug discovery program in the College of Pharmacy, and the member of BIO5 institute and the cancer center at the University of Arizona. His group research interest includes 1) New synthetic methodology development, particular asymmetric synthesis and catalysts; 2) Drug discovery and chemical biology/medicinal chemistry; and 3) Molecular recognition and imaging and drug delivery. He and his co-workers have published more than 250 papers including *Nat. Commun., Nat. Mol. Biol., J. Am. Chem. Soc.*,

Angew. Chem. etc. 1book, 16 book chapters and 5 patents with h-index 72. One of his patents has been licensed to the Aldrich Chemical Company, Inc., for his metal-free organo-catalysts technology, and one to the Andaman Therapeutics, Inc. for his bi-functional cancer drugs technology. He has received several awards including the Creative Award from the University of New Mexico (2012 and 2014), the Chinese-American Chemistry & Chemical Biology Professors Association (CAPA) Distinguished Junior Faculty Award (2008) and the American Peptide Society the Bruce W. Erickson Young Investigator Award (2001).

# Design and Fabrication of Metal Oxide Semiconductors for Photocatalytic Applications

Songling Wang and Guo Qin Xu

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Photocatalysis has attracted much attention because of its applications in environmental and energy research areas. Developing photocatalysts with rational structures is one promising way to improve photocatalytic properties. We designed and fabricated a series of metal oxide semiconductors for photocatalytic applications.

WO<sub>2</sub>/WO<sub>3</sub> hybrid nanorods were synthesized using a one-step solvothermal method. The presence of metallic WO<sub>2</sub> promotes the charge-carrier separation of WO<sub>3</sub>. This hybrid gives rise to the enhanced photocatalytic oxygen evolution activity with visible-NIR light. Two-dimensional C/TiO<sub>2</sub> heterogeneous hybrid was also prepared. Layered structure of 2-D TiO<sub>2</sub> and chemically bonded Ti-C between graphitic carbon and TiO<sub>2</sub> generate synergetic effects for interfacial charge transfer and separation, thus leading to more electrons participating in photo-reduction for hydrogen evolution. In the absence of noble metals, the C/TiO<sub>2</sub> exhibits a significant enhancement of hydrogen evolution from water splitting under solar light.

We successfully fabricated a free-standing 2-D  $\text{TiO}_2$  sheet with an optical onset of  $\sim$  1.84 eV. Using first principles calculation in combination with experiments, the asformed 2-D  $\text{TiO}_2$  sheets were found to be layers of lepidocrocite  $\text{TiO}_2$ , but with large non-uniform strains consistent with its crumpled morphology. These strains cause a significant change in the quasiparticle band structure and optical absorption spectra, resulting in large absorption in visible light region and an enhanced photocatalytic property with low-energy photons.

# Prof. Guo Qin Xu

Guo Qin Xu graduated with BSc in chemistry from Fudan University, China in 1982. He completed his PhD studies at Princeton University in 1987. He then worked as a research associate in Brookhaven National Laboratory and University of Toronto. In 1991, he joined Department of Chemistry, the National University of Singapore. His research mainly focuses on semiconductor surface chemistry and nano-materials. Currently, he is a professor in the National University of Singapore.

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