

2018



兴大报告年报

Xingda Lecture Yearbook



北京大学化学与分子工程学院

College of Chemistry and Molecular Engineering

Peking University

Preface

At the turning point to reform and boost its research and education system in 1995, College of Chemistry and Molecular Engineering (CCME) at Peking University, China, proposed to set up a science forum to foster idea refreshments and brainstorming between its faculty and outside scientists, aiming at broadening its collaborations with institutions of chemical sciences and educations all over the world. Against all odds, CCME and Beijing Xinda Scientific Systems hit it off instantly to jointly establish the Xingda Lecture Series. Thanks to its enthusiasm for science, Beijing Xinda Scientific Systems has been financially supporting this lecture series ever since then. From the very beginning, Prof. Chunhua Yan had been serving as the organizer of this lecture series until 2015 after which Prof. Kai Wu was named as the successor.

The Xingda Lecture Series is held on every Friday throughout the academic year. Up to the time this booklet was edited, about 500 scientists had been invited to give talks at the Xingda Lecture Series which nearly cover all the research areas in chemistry and related disciplines. Needless to say, this lecture series won't be able to last without great contribution from these scientists.

With the great success of the Xingda Lecture series that has already benefited the faculty and students at CCME and the science communities inside and outside PKU as well, CCME in 2015 made the decision to upgrade this forum to the Xingda Lectureship that would be held by invited renowned and distinguished scientists from all over the world. This is also echoing the mission of Peking University in the new century which is to advance sciences and cultivate next-generation scientists for the betterment of humanity. To do this, a searching committee chaired by Prof. Kai Wu was established to select and invite scientists, normally one year in advance, to spend a period of time at CCME to share their latest achievements and exchange ideas with the faculty and students at CCME through both the Xingda Lectureship and in-lab discussions.

As a thank-you gift and historical document, we have edited this booklet to record the invited speakers and their biosketches as well as the titles and abstracts of their presentations delivered at the Xingda Lectureship in the last academic year. We'll continue to do this on a yearly basis in the future.

Last but not least, we are grateful to all who have been involved in the Xingda Lectureship and helped us in one way or another.

Kai Wu



Organizer, the Xingda Lectureship
May, 2017

2018 Xingda Lecture schedule

Issue	Time	Speaker	Institution	Title
539	March, 9	Yi Cui	Stanford University	Nanotechnology for Energy, Environment and Textile
540	March, 23	Feng Shao	National Institute of Biological Sciences, Beijing	Pyroptosis: From Innate Immunity to Cancer
541	March, 30	Yingming Zhao	University of Chicago	Chemical Proteomics Approaches for discovery and characterization of New Lysine Acylation Pathways
542	April, 6	Toshikazu TAKATA	Tokyo Institute of Technology	Smart Stimuli-Responsive Materials Driven by Rotaxane Molecular Switch
543	April, 20	Jillian Buriak	University of Alberta & National Institute for Nanotechnology	Directed Self-Assembly for Nanolithography: Writing with Polymers
544	April, 27	Yushan Yan	University of Delaware	Toward Platinum-Free Fuel Cells for Affordable Zero-Emission Cars
545	May, 11	Zhengang Wang	California Institute of Technology	Electrostatics beyond Poisson-Boltzmann: Effects of Self-Energy
546	May, 18	Horst Geckeis	Institute for Nuclear Disposal & Karlsruhe Institute of Technology	Aspects of environmental actinide chemistry
547	May, 25	Xiaoyang Zhu	Columbia University	Solving the lead halide perovskite puzzle
548	June, 1	Hung-Wen Liu	University of Texas at Austin	Studies of SpnF-Catalyzed [4+2]-Cycloaddition in the Biosynthesis of Spinosyn A
549	June, 8	Javier Pérez-Ramírez	ETH	Catalysis engineering for sustainable technologies
550	September, 14	Phil S. Baran	Scripps Institute	Translational Chemistry
551	September, 21	JoAnne Stubbe	MIT	Radicals: your life is in their hands
552	October, 12	Christopher Cummins	MIT	Phosphorus-Element Bond-Forming Reactions

553	October, 12	David Leigh	East China Normal University, China; University of Manchester, United Kingdom	Making the Tiniest Machines
554	October, 19	Christopher M. Overall	University of British Columbia	N-terminomics. How TAILS Positional Proteomics Mechanistically Deciphers Pathology and led to an Allosteric Molecular Corrector Rescuing Function in an Immunodeficient Patient
555	October, 26	Ulrike Diebold	Technische Universität Wien	Surface Chemistry at the Atomic Scale
556	November, 2	Erick M. Carreira	ETH	Recent Developments in Strategies and Tactics Towards Complex Secondary Metabolites
557	November, 9	Greg Voth	University of Chicago	Overcoming the Multiscale Challenge for Biomolecular Systems
558	November, 16	Zhenan Bao	Stanford University	Overcoming the Multiscale Challenge for Biomolecular Systems
559	November, 16	George M. Whitesides	Harvard University	Future of Chemistry
560	November, 23	Yi Luo	University of Science and Technology of China	空间局域场下的单分子行为
561	November, 30	Marc A. Hillmyer	University of Minnesota	Harnessing disorder in self-assembled block polymers for functional nanostructured materials

Nanotechnology for Energy, Environment and Textile

Abstract

Nanotechnology has provided a novel technology platform which can address critical energy and environmental problems and enable new opportunities. In the past decade, my group has conducted research on innovative ideas to address problems related to energy conversion, storage and saving, and environment cleaning (air, water and soil), to create new opportunities in wearable applications. Here I will show exciting examples, including: 1) high energy battery materials including Si and Li metal anodes and S cathodes; 2) electrochemical tuning of catalysts; 3) Water disinfection using conducting nanofilters and uranium extraction for seawater. 4) Nanofiber air filters for efficient PM_{2.5} removal and low air resistance. 5) Cooling and heating textile for personal thermal management. Nanotechnology represents the most important foundational technology platform to impact nearly all areas of applications.

Prof. Yi Cui (崔屹)

Department of Materials Science and Engineering, Stanford University.
Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory.



Yi Cui is a Professor in the Department of Materials Science and Engineering at Stanford University. He received B.S. in Chemistry in 1998 at the University of Science and Technology of China (USTC), Ph.D. in 2002 at Harvard University. After that, he went on to work as a Miller Postdoctoral Fellow at University of California, Berkeley. In 2005, he became an Assistant Professor in the Department of Materials Science and Engineering at Stanford University. In 2010, he was promoted with tenure. His current research is on nanomaterials for energy storage, photovoltaics, topological insulators, biology and environment. He has founded three companies to commercialize technologies from his group: Amprius Inc., 4C Air Inc. and EEnovate Technology Inc. He is a fellow of Materials Research Society and a fellow of Royal Society of Chemistry. He is an Associate Editor of Nano Letters. He is a Co-Director of the Bay Area Photovoltaics Consortium and a Co-Director of Battery 500 Consortium. He is a highly proliferate materials scientist and has published ~390 research papers.

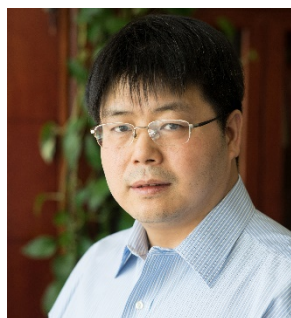
Honors and Awards

In 2014, he was ranked NO.1 in Materials Science by Thomson Reuters as “The World’s Most Influential Scientific Minds”. His selected awards include: Blavatnik National Laureate (2017), MRS Kavli Distinguished Lectureship in Nanoscience (2015), the Sloan Research Fellowship (2010), KAUST Investigator Award (2008), ONR Young Investigator Award (2008), Technology Review World Top Young Innovator Award (2004). World Top Young Innovator Award (2004).



Pyroptosis: From Innate Immunity to Cancer

Prof. Shao Feng (邵峰)



Investigator and Deputy Director
 National Institute of Biological Sciences

1991-1996 B.S., Applied Chemistry, *Peking University*, Beijing, China.
 1996-1999 M.S., Molecular Biology, *Institute of Biophysics, CAS*, Beijing, China.
 1999-2003 Ph.D., Biological Chemistry, *University of Michigan*, Ann Arbor, MI, USA
 2003-2003 Postdoctoral fellow, *University of California*, San Diego, CA, USA.
 2004-2005 Damon Runyon Postdoctoral Fellow, *Harvard Medical School*, Boston, MA

2005-2012 Assistant investigator, National Institute of Biological Sciences, Beijing

2012-present Investigator, National Institute of Biological Sciences, Beijing

2014-present Deputy Director for Academic Affairs, National Institute of Biological Sciences, Beijing

Selected Publications

1. Li P, Jiang W, Yu Q, Liu W, Zhou P, Li J, Xu J, Xu B, Wang F & Shao F (2017). *Nature*, 551(7665), 378–383
2. Wang Y, Gao W, Shi X, Ding J, Liu W, He H, Wang K & Shao F. (2017). *Nature*, 547 (7661), 99-103
3. Ding J, Wang K, Liu W, She Y, Sun Q, Shi J, Sun H, Wang DC & Shao F. (2016). *Nature*, 535 (7610), 111-116
4. Shi J, Zhao Y, Wang K, Shi X, Wang Y, Huang H, Zhuang Y, Cai T, Wang F & Shao F. (2015) *Nature*, 526(7601), 660–665.

Honors and Awards

The Zhou Guang Zhao Prize for Outstanding Youth in Basic Science, 2008, Zhao Guang Zhao Foundation, Hong Kong, China

HHMI International Early Career Award (2012-2016), Howard Hughes Medical Institute, USA

The 15th Wu Jieping-Paul Janssen Medical & Pharmaceutical Award, 2014, the International Exchange and Cooperation Center of the Ministry of Health, China.

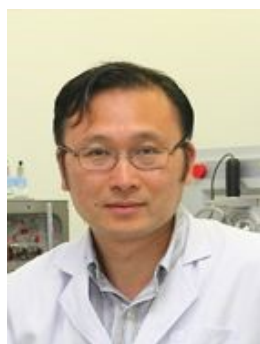
National Natural Science Funds for Distinguished Young Scholar (2013-2016).



Chemical Proteomics Approaches for discovery and characterization of New Lysine Acylation Pathways

Abstract

Iron plays a central role in the two major processes that convert nitrogen in the atmosphere to fertilizers needed for Functional characterization of thousands of small molecules in mammalian cells represents one of the major daunting challenges in biology. The cellular metabolites can activate or inhibit functions of a protein or protein complex, covalently or non-covalently. Decoding of the metabolite – protein networks would better understand cellular regulation and physiology. In this presentation, we will report our efforts to develop a systematic approach for identifying and validating new protein post-translational modifications (PTMs). We discovered lysine short-chain acylations as new types of epigenetic mechanism and as functional destination for short-chain lipids. We detected and comprehensively validated nine types of new short-chain, lysine acylation pathways: propionylation, butyrylation, crotonylation, malonylation, succinylation, glutarylation, 2-hydroxyisobutyrylation, 3-hydroxybutyrylation, and benzoylation. We identified ~500 histone marks bearing the new PTMs, which almost doubled the number of previously described histone marks that were discovered over the past few decades. We subsequently characterized the new PTM pathways by chemical proteomics and chemical biology approaches, in combination with other biological tools. Using the MS-based proteomics approach, we identified thousands of substrates for these PTM pathways, including acetyllysine and succinyllysine substrates. We and others identified regulatory enzymes that can add or remove lysine acylations. Interestingly, we showed that diverse HATs and HDACs (e.g., SIRT5) have high activities to these new lysine acylations but not lysine acetylation, suggesting that some of HDACs were mistakenly classified as deacetylases. These new PTM pathways are associated with gene expression, cellular physiology and diverse metabolic diseases. Accordingly, our study lays a foundation for studying biological functions of the short-chain metabolites and the PTM pathways, including but not limited to their roles in epigenetics and in disease.



Prof. Yingming Zhao (赵英明)

Professor, Ben May Department for Cancer Research,
The University of Chicago, Chicago, IL

10/11-present Professor, Ben May Department for Cancer Research, The University of Chicago

10/08-09/11 Associate Professor, Ben May Department for Cancer Research, The University of Chicago

02/05-09/08 Associate Professor, Department of Biochemistry, The University of Texas Southwestern Medical Center at Dallas; Co-Director, Protein Chemistry Core Center

09/00-01/05 Assistant Professor, Department of Biochemistry, The University of Texas Southwestern Medical Center at Dallas; Co-Director, Protein Chemistry Core Center

09/98-09/00 Assistant Professor; Director, Mass spectrometry Core Facility, Department of Human Genetics, The Mount Sinai School of Medicine.

08/93-03/98 Graduate Fellow and Postdoctoral Associate, Laboratory of Mass Spectrometry and Gas Phase Chemistry, The Rockefeller University



Smart Stimuli-Responsive Materials Driven by Rotaxane Molecular Switch

Abstract

Syntheses and functions of novel stimuli-responsive materials are discussed, following the brief introduction of other works achieved so far in supramolecular, organic, and polymer chemistry fields in our laboratory.

One of the most fascinating functions of polymers seems dynamic function caused by hierarchically changeable polymers as stimuli-responsive polymers which enable to enhance small structural change to bulk property change. In particular, we would like to emphasize stimulus-induced transformation of polymer topology as potential function rising in new era of polymer science, since polymer property largely depends on the polymer topology. In the present talk, we discuss mainly on the polymer topology change from linear to cyclic or from linear to star shape along with the accompanying property change. These topology changes are driven by rotaxane molecular and macromolecular switches, i.e. most reliable switch systems, where simple chemical reaction causes small partial polymer structural change which is gradually amplified to polymer shape or topology change, polymer assembly or morphology change, and finally polymer property change. From view point of practical use, we may also discuss on the development of polymer materials extraordinarily toughened by cross-linking with rotaxane cross-linkers which prove mobility of polymer chains at the cross-link points.



Prof. Toshikazu Takata

Department of Chemical Science and Engineering
 Tokyo Institute of Technology

1981	Ph. D., Tsukuba University
1981-1985	Research Associate, Tsukuba University
1985-1988	Associate Professor, Tokyo Institute of Technology
1988-1994	Full Professor, Japan Advanced Institute of Science and Technology
1995-2003	Full Professor, Osaka Prefecture University
2003- present	Full Professor, Tokyo Institute of Technology

Selected Publications

1. D. Aoki, S. Uchida, T. Takata, *Angew. Chem. Int. Ed.* 2015, 54, 6770 ~ 6774.
2. D. Aoki, S. Uchida, H. Marubayashi, S. Nojima, T. Takata, *Angew. Chem. Int. Ed.* 2016, 55, 2778 ~ 2781.
3. D. Aoki, G. Aibara, S. Uchida, T. Takata, *J. Am. Chem. Soc.* 2017, 139, 6195 ~ 6199.

Honors and Awards

The Chemical Society of Japan Award (2016), Molecular Chirality Award (2013), The Environment Award (Excellent)-The Award of Minister of Environment (2012), The CSJ Award for Technical Development (2011), The Commendation of the Minister of Education, Culture, Sports, Science and Technology (2010), The Award of the Society of Rubber Science and Technology, Japan (2009), The Award of the Society of Polymer Science, Japan (2005).



Directed Self-Assembly for Nanolithography: Writing with Polymers

Abstract

Nanopatterned surfaces are of central importance to a variety of areas and applications, such as computer chip architectures, tissue interfacing, biosensors, light management and plasmonics, among others. One of the most important materials for a myriad of functions is silicon, as the functionalization of silicon surfaces is of interest for computing applications, water splitting, batteries, on-chip sensing, molecular electronics, and solar energy conversion, amongst many others. Typically, the various approaches to nanopatterning of surfaces, including silicon, are broken into two major classes: top-down methods such as photolithography, e-beam lithography and scanning force microscopy variants, and bottom-up synthetic techniques, including self-assembly. Since lithography is the single most expensive step in computer chip manufacturing, the use of self-assembled block copolymers (BCPs) templates on surfaces is being seriously considered by the semiconductor industry to pattern, sub-20 nm features on a semiconductor surface; the Industry Technology Roadmap for Semiconductors (ITRS) terms this development 'directed self-assembly', or DSA. Here, we will describe the remarkable versatility of using BCPs, polymers that contain sufficient chemical information to form highly ordered templates over large areas. These templates, which range from arrays of parallel lines, to dots, to much more complex Moiré superlattice patterns, can be converted into functional materials, such as metal nanostructures, molecules-on-silicon, and plasmonic stamps. The versatility of using self-assembly will be combined with large-scale statistical analysis of 'quality', to better understand both the promise and limitations of this approach to nanopatterning surfaces.



Prof. Jillian Buriak

Department of Chemistry, and the National Institute for Nanotechnology, University of Alberta, Edmonton, Alberta, Canada

7/2003 - present National Institute for Nanotechnology, Canada Group Leader, National Research Council

7/2003 - present University of Alberta, Canada Professor of Chemistry and Canada Research Chair

8/2001 - 7/2003 Purdue University, West Lafayette, IN Associate professor of chemistry (with tenure)

8/1997 - 8/2001 Purdue University, West Lafayette, IN Assistant professor of chemistry

6/1995 - 6/1997 The Scripps Research Institute, La Jolla, CA Post-doctoral research associate in the laboratory of Prof. M. Reza Ghadiri

9/1991 - 5/1995 Université Louis Pasteur, Strasbourg, France Ph.D. with John Osborn (deceased)

6/1990 - 8/1990 ICI Europa, Kortenberg, Belgium Summer ICI Americas Fellow

2/1989 - 6/1990 Harvard University, Cambridge, U.S.A. Undergraduate research work with Andrew R. Barron (now at Rice University)

Honors and Awards

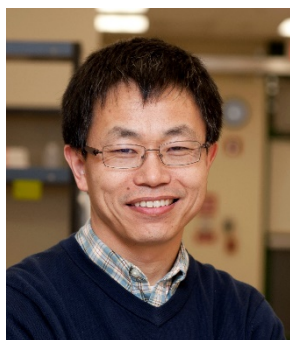
E.W.R. Steacie Award, Burghausen Chemistry Award, Canada Research Chair of Nanomaterials for Energy, Arthur Doolittle Award, Senior Fellow of the Canadian Institute for Advanced Research, Killam Annual Professorship, Alberta Innovates Industrial Research Chair, Clara Benson Award, Fellow of the American Association for the Advancement of Science, Fellow of the Royal Society of Canada, Canada Research Chair of Nanomaterials, E. W. R. Steacie Memorial Fellowship, Faculty of Science Research Prize, Martha Cook Piper Research Prize, Fellow of the Royal Society of Chemistry, Rutherford Memorial Medal in Chemistry, WISSET (Women in Science, Engineering and Technology) Fellow, Young Global Leader, World Economic Forum, Canada Research Chair of Inorganic and Nanoscale Materials and so on.

Toward Platinum-Free Fuel Cells for Affordable Zero-Emission Cars

Abstract

One of the grand challenges facing humanity today is the development of an alternative energy system that is safe, clean, and sustainable and where combustion of fossil fuels no longer dominates. A distributed renewable electrochemical energy and mobility system (DREEMS) could meet this challenge. At the foundation of this new energy system, we have chosen to study a number of electrochemical devices including fuel cells, electrolyzers, and flow batteries. For all these devices electrocatalysis and polymer electrolytes play a critical role in controlling their performance, cost, and durability, and thus their economic viability. In this presentation, I will focus on our recent work on hydroxide exchange membrane fuel cells (HEMFCs) which can work with nonprecious metal catalysts and inexpensive hydrocarbon polymer membranes. More specifically I will show the roadmap we have developed for this technology, the progress we have made in developing the most stable membranes and the most active nonprecious metal catalysts. I will also discuss why hydrogen oxidation reactions are slower in base than in acid for precious metal catalysts.

Prof. Yushan Yan (严玉山)



Distinguished Engineering Professor. Department of Chemical and Biomolecular Engineering. Associate Dean for Research and Entrepreneurship, College of Engineering, University of Delaware

Yushan Yan is the Distinguished Engineering Professor and the Associate Dean for Research and Entrepreneurship of the College of Engineering at the University of Delaware. He studied Chemical Physics (BS) at the University of Science and Technology of China, Heterogeneous Catalysis at the Dalian Institute of Chemical Physics of the Chinese Academy of Sciences, and Chemical Engineering (MS/PhD) at the California Institute of Technology. He worked for AlliedSignal as Senior Staff

Engineer and Project Leader before joining the faculty at the University of California Riverside where he served as the Department Chair.

Honors and Awards

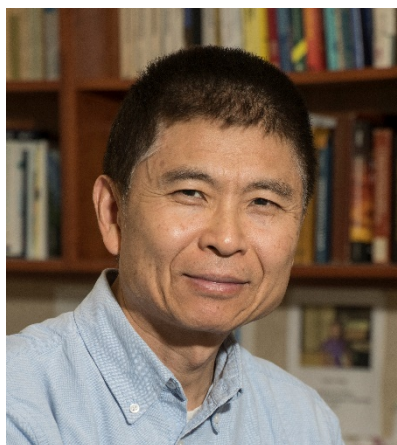
His major recognitions include Fellow of the American Association for the Advancement of Science, the Donald Breck Award from the International Zeolite Association, the Nanoscale Science and Engineering Forum Award from the American Institute of Chemical Engineers, and the Energy Technology Division Award from the Electrochemical Society. He was one of 37 awardees of the US Department of Energy's ARPA-E OPEN 2009 (1st open call for proposals) and one of 66 awardees of the ARPA-E OPEN 2012 (2nd open call for proposals). He has been an inventor on a number of issued or pending patents, some of which were licensed to form startup companies (e.g., NanoH₂O and OH-Energy). His research has led to 230+ publications that are widely cited (14,000+ citations, h-index = 64 and average citation/paper = 61) and been extensively covered by the media including New Scientist, Business Week, C&EN News, Materials Today, MRS360, Chemical Engineering Progress, China Press, Chinese Daily News, CNBC, CNN.com, KABC, Radio Australia, and VOA.



Electrostatics beyond Poisson-Boltzmann: Effects of Self-Energy

Abstract

Ions are essential in physical chemistry, colloidal science, electrochemistry, biology and many other areas of science and engineering. While their role is commonly described in terms of screening and translational entropy, many phenomena, ranging from some classical experimental observations made many decades ago to some new systems of current interest, cannot be explained, even qualitatively, by these concepts. A key effect that is often ignored or inadequately treated in the main literature on electrolytes and polyelectrolytes is the self-energy of the ions. In this talk, I will discuss several self-energy effects in macromolecular and interfacial systems. First, we show that the preferential solvation energy of the ions provides a significant driving force for phase separation. This concept is used to develop a theory to explain the dramatic shift in the order-disorder transition temperature in PEO-PS diblock copolymers upon the addition of salt. Second, we show that the dielectric contrast between the polymer backbone and the solvent significantly affects the conformation and charge condensation in dilute polyelectrolyte solutions. Third, we show that the image force has qualitative effects on the double layer structure and forces, such as like charge attraction and charge inversion. Finally, we present a simple theory for treating charge correlation effects in polyelectrolyte solutions that self-consistently account for the conformation changes of the polyelectrolyte chains.



Prof. Zhengang Wang (王振纲)

Dick and Barbara Dickinson Professor of Chemical Engineering

1982 B.Sc., Chemistry, Beijing University

1987 Ph.D., Chemistry, University of Chicago

王振纲教授是国际知名的高分子和软物质理论物理学家。主要研究领域涉及高分子溶液、混合物和共聚物的热力学与动力学；表面和界面；液晶态、胶体和凝胶；软物质体系的静电相互作用；DNA 和 RNA 的生物物理和病毒自组装；生物膜物理等。在国际核心期刊上发表研究论文一百四十余篇，多次应邀在美国化学会年会、美国物理学会年会等重大国际会议上做报告。

Honors and Awards

Braskem Award for Excellence in Materials Engineering and Science, American Institute of Chemical Engineers (2018)

Xing Da Lecturer, College of Chemistry and Molecular Engineering, Peking University (2018)

Robert Scott Lecturer, Department of Chemistry and Biochemistry, UCLA (2015)

Albert Moscowitz Lecturer, Department of Chemistry, University of Minnesota (2015)

Michael M. Abbott Lecturer, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute (2009)

Richard P. Feynman Prize for Excellence in Teaching (Caltech) (2008)

Fellow, American Physical Society (2001)

Alfred P. Sloan Award (1996)

Richard M. Badger Teaching Prize (Division of Chemistry and Chemical Engineering, Caltech) (1995)

Camille Dreyfus Teacher-Scholar Award (1995)

Visiting Research Fellow, The Institute for Advanced Studies, The Hebrew University, Jerusalem, Israel (1993)

Camille and Henry Dreyfus New Faculty Award (1991)

Aspects of environmental actinide chemistry

Abstract

Since their application in various technologies, notably in nuclear energy, actinide elements have gained significant interest by environmental scientists (e.g. [1, 2]). Besides uranium and thorium, also transuranium elements, notably plutonium, can be found in the natural environment. While the naturogenic plutonium isotopes ^{244}Pu and ^{239}Pu are only abundant at ultra-trace levels in the earth crust, anthropogenic releases between the 1950s and the 1970s via nuclear weapon tests and from military processing installations into the environment amount to more than 20 tons [3]. In addition, quite a number of countries using nuclear energy have decided to dispose spent nuclear fuel in a geological repository without separating uranium and plutonium. Understanding environmental actinide behaviour is certainly of high relevance not only to appraise actinide propagation in the biosphere but also to assess their behaviour in a deep geological repository over long time scales. It is well known, that plutonium exists in its tetravalent oxidation state in many environmental compartments and thus is considered of low mobility. This is consistent with observations made for plutonium already abundant in the environment, where e.g. plutonium deposited as weapon test fallout can be found located in narrow regions of sediment layers [3, 4]. However, formation of colloidal species, complexation with organic ligands, redox transitions have been reported to enhance the mobility of the early actinide series elements under specific conditions (e.g. [5, 6]). Respective reactions are often characterized by strong kinetic hindrances. Frequently, lanthanides, uranium or thorium are taken as surrogates for americium, neptunium and plutonium. Such analogies, though being adequate in some cases, may be misleading in other cases. Ionic radii vary and thus speciation in solution can strongly differ. The capability of forming e.g. covalent bondings significantly varies between 4f and 5f elements and within the 5f element series (see e.g. [7, 8]). Consequently, thermodynamic data and speciation schemes of chemical homologies are not always applicable, but have to be determined element specific.

Prof. Horst Geckeis



Director of the Institute for Nuclear Disposal (INE) and Professor for Radiochemistry at the Karlsruhe Institute of Technology (KIT), Institute for Inorganic Chemistry, Faculty of Chemistry and Biosciences

1985	Diploma Sc., University of Saarbrücken, Germany
1989	Ph. D., University of Saarbrücken, Germany
1993-2003	Staff scientist at the Institute for Nuclear Disposal (INE) at the Karlsruhe Research Centre (FZK)
2003-2007	Head of analytical department at INE
2008-	Director of the Institute for Nuclear Disposal (INE) at the Karlsruhe Institute of Technology (KIT); Professor for Radiochemistry at the Karlsruhe Institute of Technology (KIT), Institute for Inorganic Chemistry, Faculty of Chemistry and Biosciences

Honors and Awards

1. Since 2014 member of the Nuclear Waste Management Commission (ESK) which advises the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety (BMUB) in matters of nuclear waste management.
2. Since 2013, Chairman of the German association for repository research (DAEF)
3. Chairman of the International Steering Committee of the MIGRATION conferences (International Conference on the Chemistry and Migration Behaviour of Actinides and Fission products in the Geosphere)
4. Until 2014, Chairman of the Nuclear chemistry division of the German Chemical Society (GDCH).
5. Advisory Board Member of Radiochimica Acta.

Solving the lead halide perovskite puzzle

Abstract

Research in my group aims to understand photophysics in nano, molecular, and hybrid semiconductors and interfaces. We focus on fundamental interactions beyond the single particle approximation, and probe the dynamics of quasiparticles (excitons, polarons, polaritons, etc.) that are important to a range of optoelectronic processes, such as solar energy conversion, light emission, and polariton condensation. Following a brief introduction to my research program, I will tell one particular story – the discovery of why lead halide perovskites (LHPs) work so well in solar cells and light emitting materials. A major puzzle from recent studies on LHPs is that optoelectronic performances suggest nearly perfect semiconductors despite the unavoidable presence of defects from room temperature and solution processing. Here we explain the essential physics in this class of materials based on their disordered phonon dynamics and dielectric functions. We show that the dielectric function of a hybrid organic-inorganic lead halide perovskite (LHP) possesses combined characteristics of a polar liquid and a ferroelectric material. The latter response in the THz region may lead to dynamic and local ordering of polar nano domains by an extra electron or hole, resulting a quasiparticle which we call a ferroelectric large polaron. Compared to a conventional large polaron, the collective nature of polarization in a ferroelectric large polaron may give rise to order(s)-of-magnitude larger reduction in the Coulomb potential and introduce potential barriers to charge carrier scattering. The ferroelectric large polaron may explain the defect tolerance, low recombination rates, and slow cooling of charge carriers in lead halide perovskites, as well as providing a design principle for high performance semiconductors from nano, molecular, and hybrid materials.

Prof. Xiaoyang Zhu (朱晓阳)

Department of Chemistry, Columbia University, New York

Xiaoyang Zhu is the Howard Family Professor of Nanoscience and a Professor of Chemistry at Columbia University. He received a BS degree from Fudan University in 1984 and a PhD from the University of Texas at Austin in 1989. After postdoctoral research with Gerhard Ertl at the Fritz-Haber-Institute, he joined the faculty at Southern Illinois University as an Assistant Professor in 1993. In 1997, he moved to the University of Minnesota as a tenured Associate Professor, later a Merck endowed professor. In 2009, he returned to the University of Texas at Austin as the Vauquelin Regents Professor and served as directors of the DOE Energy Frontier Research Center (EFRC) and the Center for Materials Chemistry. In 2013, he moved to Columbia University.



Honors and Awards

His honors include a Dreyfus New Faculty Award, a Cottrell Scholar Award, a Friedrich Wilhelm Bessel Award, a Fellow of the American Physical Society, a Vannevar Bush Faculty Fellow Award from DOD, and an Ahmed Zewail Award from A. Among his professional activities, he serves on the editorial/advisory boards of *Accounts of Chemical Research*, *Science Advances*, *Chemical Physics*, and *Progress in Surface Science*, and as a scientific advisor to the Fritz-Haber-Institute of the Max-Planck Society and Shanghai Tech University.

Studies of SpnF-Catalyzed [4+2]-Cycloaddition in the Biosynthesis of Spinosyn A

Abstract

The Diels–Alder reaction is a [4+2]-cycloaddition reaction in which a cyclohexene ring is formed between a 1,3-diene and an electron deficient alkene via a single pericyclic transition state. This reaction has been proposed as a key transformation in the biosynthesis of many cyclohexene-containing secondary metabolites. Although several purified enzymes have been implicated in biotransformations that are consistent with a Diels–Alder reaction, these enzymes typically demonstrate more than one catalytic activity, leaving their specific influence on the cycloaddition step uncertain. In our studies of the biosynthesis of spinosyn A, a tetracyclic polyketide-derived insecticide from *Saccharopolyspora spinosa*, we identified a cyclase, SpnF, that catalyzes a transannular [4+2]-cycloaddition to form the cyclohexene ring in the final product. SpnF is unique, because it is the first enzyme that was characterized to specifically catalyze a [4+2]-cycloaddition without introducing any other changes to its substrate. The same cycloaddition also takes place nonenzymatically, but at a much reduced rate. If the reaction catalyzed by SpnF is a concerted process with a single pericyclic transition state, then SpnF would be the first example of a naturally occurring Diels–Alderase. In order to investigate this possibility, alpha-secondary deuterium kinetic isotope effects were measured at all points of rehybridization in the diene during both the nonenzymatic and SpnF-catalyzed [4+2]-cycloaddition reactions. This was accomplished using regiospecifically deuterated substrates and electrospray ionization, time-of-flight mass spectrometry to follow changes in deuterium enrichment of the substrate as the reaction progressed. This presentation will describe the measurement of these KIEs and offer a mechanistic discussion of their implications for understanding the SpnF catalyzed [4+2]-cycloaddition.



Prof. Hung-wen (Ben) Liu

George H. Hitchings Regents Chair in Drug Design, College of Pharmacy
 Professor of Chemical Biology & Medicinal Chemistry
 Professor of Chemistry

B.S. Tunghai University
 M.A. Columbia University
 M. Phil. Columbia University
 Ph.D. Columbia University
 NIEHS Postdoctoral Fellow, Massachusetts Institute of Technology

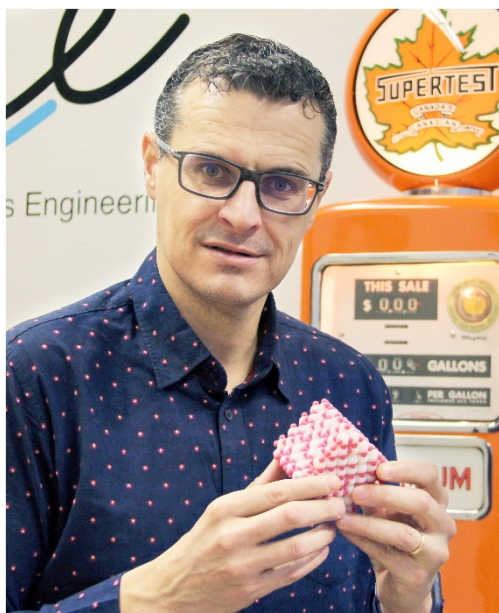
Honors and Awards

American Association for the Advancement of Science Fellow (2005)
 American Academy of Microbiology Fellow (2006)
 Japan Society for the Promotion of Science Fellow (2006)
 Nakanishi Prize, American Chemical Society, Division of Organic Chemistry (2007)
 Repligen Award in Chemistry of Biological Processes, American Chemical Society, Division of Biological Chemistry (2008)
 Elected Academician of Academia Sinica (2008)
 Tunghai University Distinguished Alumni Award (2008), Honorary Professor (2011)
 Honorary Professor, National Tsing Hua University, Taiwan (2011)
 A. I. Scott Medal for Excellence in Biological Chemistry Research (2011)
 American Chemical Society Fellow (2014)
 Arthur C. Cope Late Career Scholars Award, American Chemical Society (2014)

Catalysis engineering for sustainable technologies

Abstract

Heterogeneous catalysis is quite possibly the most relevant discipline in the chemical industry, spearheading improvements in process sustainability by improving the exploitation of raw materials, enabling the transition from fossil to renewable feedstocks, reducing energy consumption, and minimizing the environmental footprint. To confront these challenges head on, this vibrant discipline is becoming increasingly design-driven, a shift which is facilitated by the availability of increasingly powerful tools that enable the continued development of fundamental knowledge over different time and length scales. The design of a heterogeneous catalyst, a dream not long ago, is becoming a reality. In this talk, I will discuss recent examples from my laboratory to illustrate how this intellectual growth in the understanding of catalyzed processes can kindle revolutionary technological advancements.



Prof. Dr. Javier Pérez-Ramírez

ETH Zurich, Switzerland

Javier Pérez-Ramírez studied Chemical Engineering at the University of Alicante and received his PhD degree at Delft University of Technology in 2002. Following a period in industry at Norsk Hydro and Yara International (2002-2005), he joined the Institute of Chemical Research of Catalonia as an ICREA Professor before being appointed at the Swiss Federal Institute of Technology in Zurich as the Professor of Catalysis Engineering in 2010. His research focuses on the design of catalytic materials tackling current and future energy, resource, and environmental challenges of society. The main topics of interest include the valorization of renewables, carbon dioxide, and natural gas using tailored nanostructured materials. He has published over 350 articles and is co-inventor of 17 patents.

Honors and Awards

Otto-Roelen-Medal (2012),

EFCATS Young Researcher Award (2013),

Beilby Medal and Prize (2014),

RSC Sustainable Energy Award (2017).

Associate Editor of Catalysis Science and Technology and as President of SwissCat, the Catalysis section of the Swiss Chemical Society.

Translational Chemistry

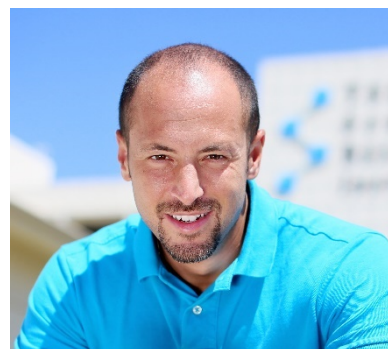
Abstract

There can be no more noble undertaking than the invention of medicines. Chemists that make up the engine of drug discovery are facing incredible pressure to do more with less in a highly restrictive and regulated process that is destined for failure more than 95% of the time. How can academic chemists working on natural products help these heroes of drug discovery – those in the pharmaceutical industry? With selected examples from our lab and others, this talk will focus on that question highlighting interesting findings in fundamental chemistry and new approaches to scalable chemical synthesis.

Prof. Phil S. Baran

The Scripps Research Institute

1997	B.S. with Honors in Chemistry, New York University
2001	Ph. D., The Scripps Research Institute, La Jolla, California
2001-2003	Postdoctoral Associate, Harvard University
2003-2006	Assistant Professor of Chemistry at The Scripps Research Institute
2006-2008	Associate Professor of Chemistry (with Tenure)
2008-	Professor of Chemistry at The Scripps Research Institute
2009-	Member, Skaggs Institute for Chemical Biology
2013-	Darlene Shiley Chair in Chemistry at The Scripps Research Institute



Selected Publications

- Horn, E. J.; Rosen, B. R.; Chen, Y.; Tang, J.; Chen, K.; Eastgate, M. D.; Baran, P. S. *Nature* **2016**, 533, 78–81.
- Kawamura, S.; Chu, H.; Felding, J.; Baran, P. S. *Nature* **2016**, 532, 90–93.
- Qin, T.; Cornella, J.; Li, C.; Malins, L. R.; Edwards, J. T.; Kawamura, S.; Maxwell, B. D.; Eastgate, M. D.; Baran, P. S. *Science* **2016**, 352, 801–805.
- Gianatassio, R.; Lopchuk, J. M.; Wang, J.; Pan, C.-M.; Malins, L. R.; Prieto, L.; Brandt, T. A.; Collins, M. R.; Gallego, G. M.; Sach, N. W.; Spangler, J. E.; Zhu, H.; Baran, P. S. *Science* **2016**, 351, 241–246.
- Lo, J. C.; Gui, J.; Yabe, Y.; Pan, C. -M.; Baran, P. S. *Nature* **2014**, 516, 343–348.

Honors and Awards

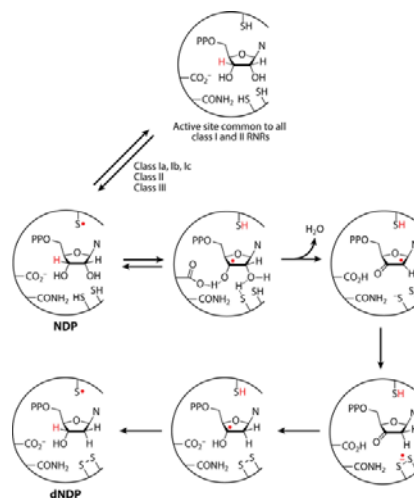
2017 Member, The National Academy of Sciences
 2016 Blavatnik National Laureate in Chemistry Award
 2016 ACS Elias J. Corey Award
 2015 Member, American Academy of Arts and Sciences
 2013 MacArthur Fellowship; 2013 Royal Society of Chemistry Synthetic Organic Chemistry Award
 2013 Fellow, Royal Society of Chemistry



Radicals: your life is in their hands

Abstract

In this talk, I will discuss the role of free radicals in biology, a problem that my lab has investigated for 30 years. Ribonucleotide reductases (RNRs) are a group of enzymes that serve as a paradigm for Nature's use of controlled radical chemistry. In all organisms, these enzymes catalyze the conversion of nucleotides, the building blocks of RNA, to deoxynucleotides, the building blocks of DNA, and consequently supply the monomeric precursors required for DNA replication and repair. While this chemical transformation, cleavage of a carbon-hydroxyl (C-OH) bond of one of four nucleotide substrates and formation of a carbon-hydrogen (C-H) bond, appears to be very "simple", nothing could be farther from the truth. The central role of RNRs in nucleic acid metabolism has also made them the successful target of three drugs that are used clinically, including gemcitabine a mechanism-based inhibitor rationally designed from our understanding of the mechanism of nucleotide reduction.



Prof. JoAnne Stubbe

Novartis Professor of Chemistry
 Professor of Biology
 MIT University



JoAnne Stubbe obtained her Bachelor degree in Chemistry in 1968 from University of Pennsylvania. She then studied Organic Chemistry as a graduate student with George Kenyon at University of California Berkeley, and obtained her Ph.D. in 1971. After graduation, she became an Assistant Professor of Chemistry at Williams College from 1971 to 1975. Then she worked Robert Abeles at Brandeis University as a Postdoctoral Fellow from 1975 to 1977. She In 1977, she joined Yale University School of Medicine as an Assistant Professor of Pharmacology. In 1980, she moved to University of Wisconsin, Madison, where she was promoted to Full Professor, and stayed until 1987. After that, JoAnne moved to MIT and became Novartis Professor of Chemistry and Professor of Biology.

Honors and Awards

American Association for the Advancement of Science, Fellow, 2014
 National Science Foundation, National Medal of Science, 2008
 National Academy of Sciences, Member, 1992
 American Academy of Arts and Sciences, Fellow, 1991
 Welch Award in Chemistry 2010
 NAS Chemical Sciences Award 2010
 Pearl Meister Greengard Award 2017



Phosphorus-Element Bond-Forming Reactions

Abstract

White phosphorus (P₄) has been the traditional entry point into phosphorus chemistry. The thirteenth element to have been isolated, it can be oxidized with elemental oxygen or chlorine, or reduced in a variety of ways. We investigated its reduction using early transition metal systems and breakdown to produce complexes with terminal metal-phosphorus triple bonds. Such terminal phosphide complexes possess nucleophilic phosphorus atoms, paving the way to new phosphorus-element bonded systems. This opened the door to the study of reactive diphosphorus molecules, the naked P₂ molecule being otherwise a high-temperature species. Subsequently, it proved possible to deliver P₂ into organic molecules using photochemical “cracking” of white phosphorus, the P₂ serving as an effective dienophile with 1,3-dienes. An alternative pathway to the generation of unsaturated, P-containing reactive intermediates is through the use of anthracene as a delivery platform as illustrated for aminophosphinidenes, the interstellar molecule HCP, and diphosphorus. The raw material serving as a phosphorus source for global agriculture is not white phosphorus, but rather apatite in phosphate rock. White phosphorus is made in the legacy “thermal process”, accounting for ca. 5% of global phosphate rock consumption but ca. 30% of the energy utilized in phosphate rock upgrading. Now we are seeking routes to value added phosphorus chemicals that leverage the “wet process”, in which phosphate rock is treated with sulfuric acid en route to phosphoric acid and phosphate fertilizers.

Prof. Christopher Colin Cummins

Department of Chemistry, Massachusetts Institute of Technology

Christopher “Kit” Colin Cummins benefited from formative undergraduate research experiences carried out sequentially in the laboratories of Professors Susan E. Kegley, James P. Collman, and Peter T. Wolczanski, respectively of Middlebury College, Stanford University and Cornell University. He graduated from the latter institution with an A.B. degree in 1989. Following this he undertook inorganic chemistry graduate studies under the direction of Professor Richard R. Schrock at the Massachusetts Institute of Technology, from which he obtained his Ph.D. degree in 1993 with a thesis entitled “Synthetic Investigations Featuring Amidometallic Complexes”. Also in 1993 Kit joined the chemistry faculty at MIT as an Assistant Professor, and in 1996 he was promoted to his current rank of Professor.



Honors and Awards

In 2007, Cummins was awarded the 2007 Raymond and Beverly Sackler Prize in the Physical Sciences by Tel Aviv University and the 2007 F. Albert Cotton Award by the American Chemical Society.

In 2008, Cummins was elected a fellow of the American Academy of Arts & Sciences.

In 2013, Cummins was awarded the Ludwig Mond Award by the Royal Society of Chemistry.

In 2017, Cummins was elected as a member of the National Academy of Sciences. In the same year, the American Chemical Society awarded Cummins the 2017 Linus Pauling Medal in recognition of his synthetic and mechanistic studies of early-transition metal complexes.



Making the Tiniest Machines

Abstract

Over the past two decades some of the first examples of synthetic molecular level machines and motors—all be they primitive by biological standards—have been developed. Perhaps the best way to appreciate the technological potential of controlled molecular-level motion is to recognise that nanomotors and molecular-level machines lie at the heart of every significant biological process. When we learn how to build artificial structures that can control and exploit molecular level motion, and interface their effects directly with other molecular-level substructures and the outside world, it will potentially impact on every aspect of functional molecule and materials design.



Prof. David Leigh

University of Manchester

1984 B. Sc., University of Sheffield,

1987 Ph. D., University of Sheffield,

2001-2012 Forbes Chair of Organic Chemistry, University of Edinburgh

2012-2013 Professor of Organic Chemistry, University of Manchester

2014- Sir Samuel Hall Chair of Chemistry, University of Manchester

Selected Publications

1. Sundus Erbas-Cakmak, Stephen D. P. Fielden, Ulvi Karaca, David A. Leigh, Charlie T. McTernan, Daniel J. Tetlow, Miriam R. Wilson. *Science* **2018**, 358, 340.
2. Salma Kassem, Alan T. L. Lee, David A. Leigh, Vanesa Marcos, Leoni I. Palmer & Simone Pisano, *Nature* **2017**, 549, 374.
3. Jonathan J. Danon, Anneke Krüger, David A. Leigh, Jean-François Lemonnier, Alexander J. Stephens, Iñigo J. Vitorica-Yrezabal, Steffen L. Woltering. *Science* **2017**, 355, 159.

Honors and Awards

- 2018 1000 Talents ‘Topnotch Talent’ Professor;
- 2017 Royal Society of Chemistry Perkin Prize for Organic Chemistry;
- 2014 Royal Society of Chemistry Pedler Award;
- 2013 ERC Advanced Grant;
- 2013 Royal Society Bakerian Medal;
- 2010 Royal Society of Chemistry Tilden Prize.



N-terminomics. How TAILS Positional Proteomics Mechanistically Deciphers Pathology and led to an Allosteric Molecular Corrector Rescuing Function in an Immunodeficient Patient

Abstract

To specifically enrich for mature protein N-termini and neo-N-termini of proteins we developed 6 and 10-plex TMT TAILS (Terminal Amine Isotopic Labeling of Substrates) (Nature Biotech 28, 281-288 (2010); Nature Protocols 6, 1578-1611 (2011)). In analyzing the N-terminome of normal human tissues we find that the N-termini of protein chains *in vivo* can commence at many points C terminal to the predicted start site and result from proteolytic processing to generate stable protein chains: Proteolytic processing generates new protein species with characteristic neo-N termini that are frequently accompanied by altered half-lives, function, interactions and location. We used TAILS to mechanistically dissect a severe human immunodeficiency disease.

The paracaspase MALT1 proteolytic activity and its molecular scaffolding are central for transducing lymphocyte antigen receptor activation of NF- κ B with unregulated MALT1 activity leading to B cell lymphomas and autoimmune disease. We developed nanomolar, selective allosteric inhibitors of MALT1 paracaspase activity that bind by replacing the side chain of Trp580 and locking the protease in an inactive conformation. Interestingly, we had previously identified a patient homozygous for a hypomorphic *MALT1* mutation suffering from combined immunodeficiency who carries a serine mutation at Trp580. We used TAILS, the N-terminal *positional proteomics* approach to compare lymphocytes from the *MALT1^{mut/mut}* patient with healthy *MALT1^{+ /mut}* family members and normal individuals using 10-plex Tandem Mass Tag in the N-terminomics TAILS approach with MS3 synchronous peak selection quantification, with and without B Cell receptor stimulation. From the MALT1 cleaved neo-N terminal peptide (prime side) and the natural N terminus of HOIL1 identified by TAILS, and the nonprime side of the HOIL1 cleavage site identified by preTAILS shotgun proteomics, we identified HOIL1 of the linear ubiquitin chain assembly complex (LUBAC) as a novel MALT1 substrate. Upon B and T cell receptor stimulation HOIL1 cleavage resulted in disassembly of LUBAC and loss of linear ubiquitination in T and B cells that prevented reactivation of NF- κ B signaling. However, in this immunodeficiency, the Trp580Ser mutation weakened the interaction between the paracaspase and C-terminal immunoglobulin domains resulting in protein instability (T_m 46.1°C *versus* 52.3°C) and consequently reduced MALT1 function and protein levels. The new allosteric inhibitors also bind MALT1-Trp580Ser, stabilizing the mutant protein and increasing the T_m to that of wild-type MALT1. Allosteric, but not MALT1 active site inhibition of patient *MALT1^{mut/mut}* lymphocytes restored MALT1 protein levels *in vivo* and rescued NF- κ B and JNK signaling. Following compound washout, MALT1 substrate cleavage was also rescued. Thus, a low molecular weight compound can rescue an enzyme deficiency by substituting for the mutated residue, inspiring potential novel precision therapies to increase mutant enzyme activity.



Prof. Christopher M. Overall

Centre for Blood Research, University of British Columbia, Canada

Dr. Overall is a Professor and Tier 1 Canada Research Chair in Proteinase Proteomics and Systems Biology at the University of British Columbia, Centre for Blood Research. He completed his undergraduate, Honors Science and Masters degrees at the University of Adelaide, South Australia; his Ph.D. in Biochemistry at the University of Toronto; and was a MRC Centennial Fellow in his post-doctoral work with Dr. Michael Smith, Nobel Laureate, Biotechnology Laboratory, University of British Columbia (UBC). On Sabbatical in 1997-1998 he was a Visiting Senior Scientist at British Biotech Pharmaceuticals, Oxford, UK and in 2004/2008 he was a Visiting Senior Scientist at the Expert Protease Platform, Novartis Pharmaceuticals, Basel, Switzerland. At the Freiburg Institute for Advanced Studies, Albert-Ludwigs Universität Freiburg, Germany he was an External Senior Fellow, and in November 2014 was appointed as an Honorary Professor, Albert-Ludwigs-Universität Freiburg.

Surface Chemistry at the Atomic Scale

Abstract

Our understanding of metal oxides has benefitted tremendously from the application of surface science techniques. Particularly useful has been Scanning Probe Microscopy, which allows to directly inspect, and even manipulate, atomic-size defects and defect-related surface chemistry. Equally important has been the development of suitable model systems, i.e., (ultra)thin films and well-prepared oxide single crystals that allow a reliable experimental and theoretical modeling with crisp and unequivocal insights into fundamental processes and mechanisms.

In the talk, recent developments in the field will be illustrated by examples including our group's recent research results on binary and ternary metal oxides. Emphasis will be laid on giving an overview of different aspects, such as the importance of the relationship between bulk and surface defects, the opportunities and the challenges of extending surface science to more complex materials and to high-pressure and aqueous environments.



Prof. Ulrike Diebold

Institute of Applied Physics, TU Wien, Vienna, Austria

Ulrike Diebold received her PhD degree in engineering physics in 1990 from the University of Technology (TU Wien) in Vienna, Austria. After working as a post-doc with Prof. Ted Madey at Rutgers University in New Jersey, she joined the faculty at Tulane University, New Orleans, U.S.A. In 2010 she returned to her alma mater, where she currently holds a full professorship at the Institute of Applied Physics.

Diebold conducts research in experimental surface science with an emphasis on metal oxide surfaces. She is particularly interested in the atomic-scale properties of these complex materials, and in unraveling their (defect)structure/reactivity relationship. The main tool, Scanning Probe Microscopy, is complemented by area-averaging surface spectroscopies and first-principles calculations.

Honors and Awards

Diebold has published more than 200 peer-reviewed articles, and has given over 300 invited talks. Her articles have been cited more than 20,000 times. She has been elected a Fellow of AVS, APS, and AAAS, and is a member of the Austrian, German, and European Academies of Sciences.

In 2015 she was awarded the Blaise Pascal medal in Materials Sciences by the European Academy of Sciences for "Surfaces of Metal Oxides, Studied at the Atomic Scale". She held the 2015 Debye Lecture entitled "Surface Science Studies of an Iron Oxide Model Catalyst" at Utrecht University, The Netherlands. Also, in 2015, on 24 November, she gave the 21st Annual Schrödinger Lecture at Trinity College Dublin, Ireland, with the title "An Atomic-Scale View at Oxide Surfaces". On 11 June 2015 she gave the R. Brdička memorial lecture at the J. Heyrovský Institute of Physical Chemistry, Prague, entitled "Surface Science of Metal Oxides".

She was awarded the Wittgenstein Award in 2013.

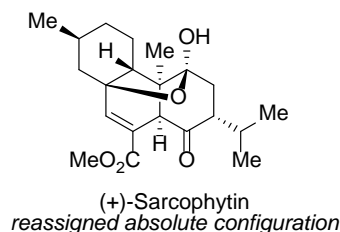
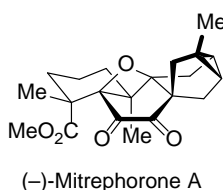
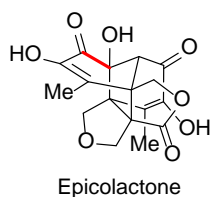
Ulrike Diebold was awarded an Advanced Grant by the European Research Council in 2011 for work on "Microscopic Processes and Phenomena at Oxide Surfaces and Interfaces".

Ulrike Diebold was elected a member of the Leopoldina, the national academy of sciences in Germany, in 2015. She was elected member of the European Academy of Sciences in 2014. In 2014, she also became an Elected Full Member of the Austrian Academy of Sciences.

Recent Developments in Strategies and Tactics Towards Complex Secondary Metabolites

Abstract

The talk will include discussion and analysis of recent natural product targets that have been synthesized in the group. It will focus on target-oriented synthesis as an engine for the generation of novel methods and approaches to bioactive agents. The methods involve novel, unexpected reactivity and unusual building blocks that are fully integrated to lead to efficient routes. Discoveries at the interface with biology serve to highlight new opportunities for target-oriented synthesis.



Prof. Erick M. Carreira

ETH Zürich

Dep. of Chemistry and Applied Biosc.

Professor Carreira obtained a B.S. degree in 1984 from the University of Illinois at Urbana-Champaign under the supervision of Scott E. Denmark and a Ph.D. degree in 1990 from Harvard University under the supervision of David A. Evans. After carrying out postdoctoral work with Peter Dervan at the California Institute of Technology through late 1992, he joined the faculty at the same institution as an assistant professor of chemistry and subsequently was promoted to the rank of associate professor of chemistry in the Spring of 1996, and full Professor in Spring 1997.

Honors and Awards

Professor Carreira is the recipient of the American Chemical Society Award in Pure Chemistry, Nobel Laureate Signature Award, Fresenius Award, a David and Lucile Packard Foundation Fellowship in Science, Alfred P. Sloan Fellowship, Camille and Henry Dreyfus Teacher Scholar Award, Merck Young Investigator Award, Eli Lilly Young Investigator Award, Pfizer Research Award, National Science Foundation CAREER Award, Arnold and Mabel Beckman Young Investigator Award, and a Camille and Henry Dreyfus New Faculty Award. He is also the recipient of the Associated Students of the California Institute of Technology Annual Award in Teaching and a Richard M. Badger Award in Teaching.



Overcoming the Multiscale Challenge for Biomolecular Systems

Abstract

A multiscale theoretical and computational methodology will be discussed that can successfully describe biomolecular systems across multiple length and time scales. The overall approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the approach is a method for deriving coarse-grained models from protein structures and their underlying molecular-scale interactions. This particular aspect of the work has strong connections to the theory of renormalization, but it is more broadly developed and implemented for heterogeneous biomolecular systems. A critical component of the methodology is also its connection to experimental structural data such as cryo-EM or x-ray, thus making it “hybrid” in its character. Important applications of the multiscale approach to study key features of large multi-protein complexes such as the HIV-1 virus capsid, the actin-based cytoskeleton, and protein-mediated membrane remodeling will be presented as time allows.



Prof. Gregory A. Voth

Department of Chemistry, James Franck Institute, and Institute for Biophysical Dynamics, University of Chicago, Chicago, IL, USA

1981 B. S., University of Kansas
 1987 Ph. D., Caltech
 1987-1989 IBM Postdoc Research Fellow, University of California, Berkeley
 1989-1996 Assistant/Associate Professor, University of Pennsylvania
 1997-2010 Distinguished Professor, University of Utah
 2010- Haig P. Papazian Distinguished Service Professor University of Chicago

Selected Publications

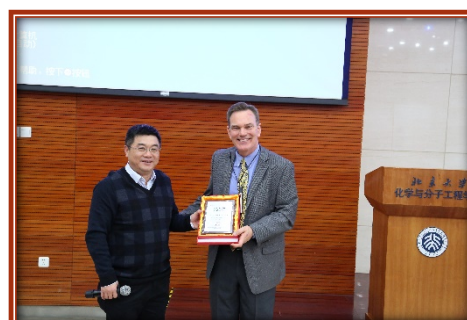
Izvekov, S.; Voth, G. A. “A Multiscale Coarse-Graining Method for Biomolecular Systems,” *J. Phys. Chem. B* 2005, 109, 2469-2473

McCullagh, M.; Saunders, M. G.; Voth, G. A. “Unraveling the Mystery of ATP Hydrolysis in Actin Filaments” *J. Am. Chem. Soc.* 2014, 136, 13053–13058

Grime, J. M. A.; Dama, J. F.; Ganser-Pornillos, B. K.; Woodward, C. L.; Jensen, G. J.; Yeager, M.; Voth, G. A. “Coarse-grained Simulation Reveals Key Features of HIV-1 Capsid Self-Assembly”, *Nature Comm.* 2016, 7, 1156

Honors and Awards

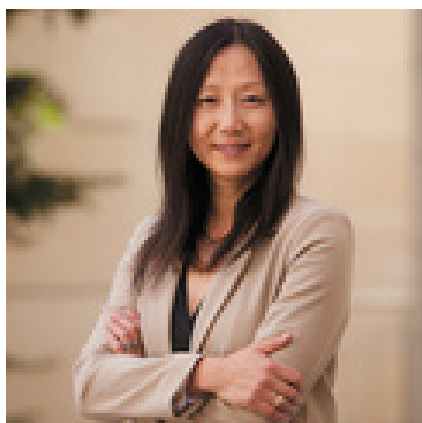
Member, International Academy of Quantum Molecular Science; ACS Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids; ACS Physical Chemistry Division Award in Theoretical Chemistry; Fellow, Biophysical Society; ACS; AAAS; APS; Stanislaw M. Ulam Distinguished Scholar, Los Alamos National Laboratory; NSF Presidential Young Investigator Award; Camille Dreyfus Teacher-Scholar Award; Alfred P. Sloan Foundation Research Fellow, David and Lucille Packard Foundation Fellow.



Skin Inspired Electronics

Abstract

Electronic devices that mimic the properties of skin have potential important applications in advanced robotics, prosthetics, and health monitoring technologies. Methods for measuring tactile and temperature signals have progressed rapidly due to innovations in materials and processing methods. Imparting skin-like stretchability to electronic devices can be accomplished by patterning traditional electronic materials or developing new materials that are intrinsically stretchable. The incorporation of sensing methods with transistors facilitates large-area sensor arrays. While sensor arrays have surpassed the properties of human skin in terms of sensitivity, time response, and device density, many opportunities remain for future development.



Prof. Zhenan Bao (鲍哲南)

Department of Chemical Engineering, Stanford University, USA

1987 B. S., Nanjing University
 1991 B. S., University of Illinois
 1993 MS, Ph.D., University of Chicago
 2001 Technical Staff, Bell Labs, Lucent Technologies
 2012 Professor, Stanford University

Selected Publications

1. S. Wang, J. Xu, Z. Bao, et al. *Nature*, 2018, 555, 83
2. Y. Kim, A. Chortos, Z. Bao, et al. *Science*, 2018, 360, 998
3. V. R. Feig, H. Tran, M. Lee, Z. Bao, *Nature Comm.*, 2018, 9, 2740
4. J. Kang, D. Son, Z. Bao, et al. *Adv. Mater.*, 2018, 30, 1706846

Honors and Awards

Wilhelm Exner Medal presented by Austrian Federal Minister of Science, 2018
 American Chemical Society (ACS) Applied Polymer Science Award, 2017.
 L’Oreal UNESCO Women in Science Award in Physical Science, 2017.
 Nature’s 10, “Master of Materials”, top ten people who mattered in 2015.
 National Academy of Engineering as Top 100 Young Engineers, 2000.



Future of Chemistry

Abstract

Like biology and biomedicine, physics and astronomy, chemistry also have its unique identity. Although chemistry has been invented for hundreds of years, there remaining a large number of problems to be solved. Now it is time to reinvent the chemistry, and new chemical problems can be roughly divided into two types, the one is intellectual problems about life, water, megacities, etc., the other one is practical problems about energy, healthcare, heterogeneous catalysis, etc. In the new era of chemistry, chemists have to think about four questions: “What are you doing?”, “Why are you doing it?”, “Your aspiration is?”, “Who cares?” In other words, the future of chemistry is closely associated with practical applications.

Prof. George M. Whitesides

Department of Chemistry and Chemical Biology, Harvard University

- 1960 B. S., Harvard University,
- 1964 Ph.D., California Institute of Technology (with J.D. Roberts),
- 1963 faculty, Massachusetts Institute of Technology
- 1982 Professor, Harvard University



Selected Publications

1. Rothmund, P., Ainla, A., Belding, L., Whitesides, G. M., et al., *Science Robotics*, **2018**, 3, 1.
2. Belding, L., Baytekin, B., Baytekin, H. T., Rothmund, P., Verma, M. S., Nemiroski, A., Grzybowski, B. A., and Whitesides, G. M., *Adv. Materials*, 2018, 30, 1704446.
3. Sharma, U., Concagh, D., Core, L., Kuang, Y., You, C., Pham, Q., Zugates, G., Busold, R., Langer, R., Whitesides, G. M., and Palasis, M., *Nature Materials*, **2018**, 17, 96.

Honors and Awards

- Alfred P. Sloan Fellowship (1968)
- American Chemical Society (ACS) Award in Pure Chemistry (1975)
- R&D Magazine’s Scientist of the Year (2007)
- Popular Mechanics Breakthrough Award (2009)
- 100 Most Creative People, FAST Company (2009)
- Gold Medal (Industrial Research Institute) (2013)



空间局域场下的单分子行为

Abstract

激发一个金属纳米腔可以产生空间高度局域的等离激元 (nanocavity plasmon, NCP), 这是一个已经被人们熟知的物理现象。在这个报告中, 我将介绍近年来我们利用 NCP 所获得的一系列新奇的现象和结果。首先, 我们发现 NCP 具有强场、超快的特性, 可以有效的改变分子发光的颜色, 利用其相干性, 我们预言并实现非线性电子散射这一全新的物理过程, 实现分子间偶极能量转移过程的空间成像。而 NCP 的空间高度局域特性, 使得我们实现了超高分辨的分子拉曼成像, 首次用光学手段看到一个分子的空间结构。局域场下与物质相互作用的描述必须超越现有的理论框架。我们发展的局域场新理论重现了实验观察的图像, 并提出了利用非共振拉曼过程, 实现分子振动模式的实空间成像的新方案。我们还进一步预言, NCP 可以产生高频磁场, 打破现有的自旋跃迁选择规则, 从而为研究分子暗态提供全新的工具。纳腔等离激元集强电场、强磁场、超快、相干、空间高度局域等特性为一体, 具有广泛的应用前景。此外金属针尖在分子催化反应中的应用, 也将给予简单的介绍。



Prof. Luo Yi (罗毅)

Professor in Theoretical Chemistry at the School of Biotechnology, KTH.
 Director of Hefei National Laboratory for Physical Sciences at the Microscale administrated by the University of Science and Technology of China (USTC).

His research group focus on the theoretical modeling of molecular electronics, nano-photonics, X-ray spectroscopies and photocatalysis. He has been collaborating with many leading experimental groups around the world. Many research results are published in the most prestigious journals in related fields, such as Nature, Nature Series, PNAS, JACS, PRL and others. Luo Yi came to Sweden in 1989 and worked at the ESCA-LASER Laboratory of Nobel Laureate, Prof. Kai Siegbahn, at Uppsala University. Luo Yi received his PhD in computational physics at Linköping University in 1996. He was employed as an Assistant Professor in Stockholm University in 1997, then became an Associated Professor in 2000 and a full Professor in 2005 at KTH. In 2010, he was awarded the Göran Gustafsson Prize in Chemistry by the Royal Swedish Academy of Sciences.

Honors and Awards

首批“千人计划”入选者(2008)和国家特聘专家, 国家杰出青年基金获得者(2009), 科技部国家重大科学研究计划项目(2010)和重点研发计划专项(2017)、国家基金委重大项目(2018)和重点项目(2016)等项目负责人。获得2010年瑞典皇家科学院“Goran Gustafsson”化学奖, 2014年作为主要完成人之一获中国科学院“杰出科技成就集体奖”。在国际学术期刊发表论文四百多篇, 被引一万三千多次, H 因子 57。



Harnessing disorder in self-assembled block polymers for functional nanostructured materials

Abstract

Self-assembled block polymers containing functional macromolecular components are versatile precursors to useful nanostructured materials. An interesting morphology used to generate nanostructured soft materials in this way is the double gyroid. The gyroid phase has the attractive feature of being bicontinuous and thus nanostructure orientation is not needed to achieve domain continuity while retaining a supporting mechanical phase. These features can be particularly useful for numerous membrane-based applications such as in ultrafiltration, photovoltaics, and polymeric electrolytes. While we have been able to access the bicontinuous double gyroid phase in, for example, polystyrene-block-poly lactide copolymers, etching those structures results in nanoporous materials that are not mechanically robust. Moreover, the gyroid structure can only be accessed over a small slice of composition in the diblock copolymer morphology map. Thus, we have worked to access block polymer nanostructures that are bicontinuous and mechanically robust but that do not necessitate the formation of the gyroid or other related ordered morphologies. I will discuss our recent approaches to nanostructured, bicontinuous disordered morphologies through either thermal or light-induced chemical fixation of block polymers in the disordered state in close proximity to the order-disorder transition. This will include our recent work on (i) how we use the in situ and controlled formation of crosslinked block polymers to trap an emerging disordered state and (ii) how we use the thermally accessible order-disorder transition to decouple the formation of a disordered phase and chemical fixation. In both cases, composition fluctuations in disordered block polymers can be trapped. In the examples where one of the blocks is chemically etchable (e.g., polylactide), nanoporous polymers with narrow pore size distributions can be generated and utilized as, for example, ultrafiltration membranes for water purification. I will focus on the preparation, characterization and applications of this interesting class of nanostructured materials.



Prof. Marc A. Hillmyer

University of Minnesota, Department of Chemistry
McKnight Presidential Endowed Chair, University of Minnesota
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Editor-in-Chief, *Macromolecules*

Marc Hillmyer received his B.S. in Chemistry from the University of Florida in 1989 and his Ph.D. in Chemistry from the California Institute of Technology in 1994. After completing a postdoctoral research position in the University of Minnesota's Department of Chemical Engineering and Materials Science he joined the Chemistry faculty at Minnesota in 1997. He is currently the McKnight Presidential Endowed Chair in Chemistry and leads a research group focused on the synthesis and self-assembly of multifunctional polymers. In addition to his teaching and research responsibilities, Marc served as an associate editor for the ACS journal *Macromolecules* from 2008-2017 and is currently the editor-in-chief of *Macromolecules*. He is also the director of the Center for Sustainable Polymers headquartered at the University of Minnesota, a National Science Foundation Center for Chemical Innovation.

Honors and Awards

McKnight Presidential Endowed Chair, University of Minnesota (UMN), 2015
NSF Division of Materials Research, Special Creativity Extension, 2014-2015 Postbaccalaureate, Graduate, and Professional Education Award (UMN), 2014
PTN Medema Award, 2013
LE STUDIUM research fellow, Université d'Orléans/CNRS, 2012-2013
Fellow of the Polymer Chemistry (POLY) Division of the American Chemical Society (ACS), 2012
Carl S. Marvel Creative Polymer Chemistry Award (POLY division of the ACS), 2011

