兴大报告 2016 年报

Yearbook of 2016

北京大学化学与分子工程学院
College of Chemistry and Molecular Engineering, Peking University

北京大学化学学院科研办公室

2017 年 5 月

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As a thank-you gift and historical document, we have edited this booklet to record the invited speakers and their biosketches as well as the titles and abstracts of their presentations delivered at the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

2016 Xingda Lecture

Issue	Time	Speaker	Institution	Title
488	Mar. 18	Zhenfeng Xi	Peking University	双金属有机合成试剂化学
489	Mar. 25	Zhongfan Liu	Peking University	刘言扉语 —— 从科学研究的 ABC 说起
490	Mar. 25	Thomas P. Russell	University of Massachusetts in Amherst	Toward Long-Range Order in Thin Films of Block Copolymers
491	Apr. 8	Manfred Scheer	University of Regensburg	The Magic of Polypnictogen Compounds
492	Apr. 22	Claudio Luchinat	University of Florence	Metabolomics by NMR: a potential revolution in diagnosis
493	Apr. 29	Mark Welland	Cambridge University	From imaging atoms to understanding human disease
494	May 20	F. N. Castellano	North Carolina State University	Photochemical Upconversion And New Frontiers In Triplet Sensitization
495	May 27	Leonard J. Foster	University of British Columbia	Interactome disassembly during apoptosis occurs independent of caspase cleavage
496	Sep. 16	Itamar Willner	Hebrew University of Jerusalem	DNA Nanotechnology: From Basic Principles to Applications
497	Sep. 16	Carolyn Bertozzi	Stanford University	Cancer Immune Therapy Targeting the Tumor Glycocalyx
498	Sep. 23	Matthew Tirrell	University of Chicago	Protein Analogous Micelles: Versatile, Modular Nanoparticles
499	Sep. 23	Xiaodong Zou	Stockholm University	Probing the 3D structures by transmission electron microscopy and electron diffraction - from zeolites and MOFs to proteins
500	Sep. 30	Jianhua Lin	Peking University	北京大学研究生教育的再思考

501	Sep. 30	David Manolopoulos	University of Oxford	From ring polymer molecular dynamics to spin dynamics
502	Oct. 14	Maria Flytzani-Stephanopoulos	Tufts University	Heterogeneous Single-Atom Metal Catalysts for Efficient Fuel Processing and Green Chemicals Production
503	Oct. 21	Shin-ichi Orimo	Tohoku University	Research Diversity on Complex Hydride
504	Oct. 21	Gregory C. Fu	California Institute of Technology	Metal-Catalyzed Cross-Couplings of Alkyl Electrophiles
505	Nov. 4	Kazunori Kataoka	The University of Tokyo	Supramolecular Nanosystems for Smart Diagnosis and Therapy of Intractable Diseases
506	Nov. 11	Andrea Hirsch	University of Erlangen - Nürnberg	Chemical Functionalization of Synthetic Carbon Allotropes
507	Nov. 11	Arieh Warshel	University of Southern California	Modeling the Action of Complex Biological Systems on a molecular Level
508	Nov. 18	Peidong Yang	UC Berkeley	$CO_2 + H_2O$ + Sunlight → Chemical Fuels + O_2
509	Nov. 18	Masafumi Unno	Gunma University	How to make well-defined silicone materials: Recent new synthetic methods
510	Dec. 2	Geert-Jan Boons	University of Georgia	Functional Glycomics Through Chemical Synthesis
511	Dec. 9	Martin Grubele	UIUC	Protein dynamics: from computer, to test tube, to the cell
512	Dec. 9	Shouheng Sun	Brown University	Tuning Nanoparticle Catalysis for Efficient Electrochemical Reactions

双金属有机合成试剂化学

Abstract

金属有机化合物作为合成试剂广泛应用于合成化学有关的各个领域，新型金属有机合成试剂的创制也因此一直受到学术界和工业界的极大关注。常见的金属有机试剂如有机锂试剂、格氏试剂等都是单金属试剂。我们研究发现，在有机桥联的配合下，存在于一个分子中的两个碳-金属键将产生“协同效应”，表现出不同于其相应单金属试剂的反应类型，甚至表现出全新的反应模式。我们将该类化合物统称为“双金属有机合成试剂”(Organo-di-Metallic reagents)。本次报告将简要介绍双金属有机试剂独特的反应化学和机制，重点介绍我们利用丁二烯基双锂试剂的氧化还原活性合成芳香性金属杂环的新进展。

Prof. Zhenfeng Xi (席振峰 院士)

College of Chemistry and Molecular Engineering, Peking University
1983 B.Sc., Xiamen University
1989 M.Sc., Nanjing University, Zhengzhou University, Henan Institute of Chemistry
1996 Ph.D., Institute for Molecular Sciences (IMS), Japan
1996-1997 Postdoctoral Research Fellow, Catalysis Research Center (CRC), Hokkaido University, Japan
1997-1998 Assistant Professor, Hokkaido University, Japan
1998-1999 Associate Professor, Peking University
1999- Professor, Peking University

Selected Publications

1. Xi, Z., *Acc. Chem. Res*. **2010**, *43*, 1342-1451.
2. Zhang, W. -X.; Zhang, S.; Xi, Z., *Acc. Chem. Res.* **2011**, *44*, 541-551.
3. Zhang, S.; Zhang, W. -X.; Xi, Z., *Acc. Chem. Res.* **2015**, in press.
4. Hao, W.; Wei, J.; Geng, W.; Zhang, W. -X.; Xi, Z., *Angew. Chem. Int. Ed.* **2014**, *53*, 14533-14537.
5. Wei, J.; Zhang, W. -X.; Xi, Z., *Angew. Chem. Int. Ed.* **2015**, *54*, 5999-6002.

Honors and Awards

1998 National Science Fund for Distinguished Young Scholars of NSFC 2000 Young Investigator Award from Hong Kong Qiu Shi Science & Technologies Foundation 2002 Cheung Kong Professor (Ministry of Education) 2003 CCS-BASF Innovation Prize 2004 Yaozeng Huang Organometallic Chemistry Award 2005 Eli Lilly Research Excellence Award in China 2006 PKU Zheng-Da Teaching Award (1st class) 2006 Visiting Professor at Hokkaido University, Japan 2007 Wuxi Pharma Tech Life Science and Chemistry Award (1st class) 2007 Visiting Professor at University of Rennes 1, France 2010 Visiting Principal Investigator at RIKEN, Japan 2014 CCS-AkzoNobel Chemical Sciences Award 2015 Academic Divisions of the Chinese Academy of Sciences

刘言雇语 —— 从科学研究的 ABC 说起

Prof. Zhongfan Liu (刘忠范 院士)

College of Chemistry and Molecular Engineering, Peking University
1983 B.Eng., Changchun Institute of Technology
1987 M.Sc., Yokohama National University
1990 Ph.D., University of Tokyo
1991-1993 Postdoctoral Research Fellow, University of Tokyo and Institute for Molecular Science
1993- Associate Professor (93.6) and Professor (93.8), Peking University
Webpage: www.chem.pku.edu.cn/nanochemistry

Selected Publications

1. Gao, T.; Song, X.; Du, H.; Nie, Y.; Chen, Y.; Ji, Q.; Sun, J.; Yang, Y.; Zhang Y.; Liu Z., *Nature Comm.* **2015**, *6*, 6835.
2. Zhang, L.; Yu, J.; Yang, M.; Xie, Q.; Peng, H.; Liu, Z., *Nature Comm.* **2013**,*4,*1443.
3. Yan, K.; Wu, D.; Peng H.; Jin, L.; Fu, Q.; Bao, X.; Liu, Z., *Nature Comm.* **2012**, *3*, 1280.
4. Peng, H.; Dang, W.; Cao, J.; Chen, Y.; Wu, D.; Zheng, W.; Li, H.; Shen, Z.; Liu, Z., *Nature Chemistry* **2012**, *4*, 281.
5. Liao, L.; Peng, H.; Liu, Z., *J. Am. Chem. Soc.* **2014**, *136*, 12194.

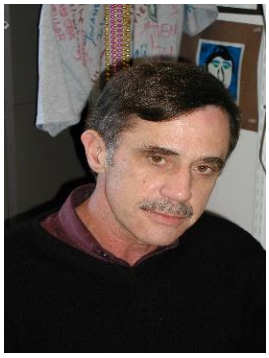
Honors and Awards

1999 Cheung Kong Professorship, 2008 National Natural Science Award 2nd Class, 2011 Academician, 2012 Chinese Chemical Society-AkzoNobel Chemical Science Award, 2013 Outstanding Scientist selected by Ten-Thousand-Talents Program, Fellow of Royal Society of Chemistry(UK), Fellow of Institute of Physics(UK)

Toward Long-Range Order in Thin Films of Block Copolymers

Abstract

Perfecting in the lateral order in thin films of block copolymers holds promise for the generation of ultra-high areal density nanostructured materials with potential applications as storage media, displays and meta-materials. Yet, achieving the needed perfection in the ordering has been elusive. Thermal and solvent annealing processes and combinations of the two have been used. Here, we will present results on solvent annealing and thermal annealing and provide a comparison between the two, outlining the advantages and disadvantages and present possible routes by which a perfection in the ordering can be achieved.



Prof. Thomas Russell

Polymer Science and Engineering Department, University of Massachusetts in Amherst

1976 B. Sc., Boston State College
1976 M. Sc., University of Massachusetts, Amherst
1979 Ph. D., University of Massachusetts, Amherst
1979-1981 Research Associate, University of Mainz
1981-1996 Research Staff, IBM Almaden Research Center
1997-present Professor, University of Massachusetts Amherst
Web: https://www.pse.umass.edu/faculty/researchgroup/russell

Selected Publications

1. Cui, M.; Emrick, T.; Russell, T. P., *Science* **2013**, *342*(6157), 460-463.
2. Russell, T. P., *Science* **2013**, *341*(6152), 1351-1352.
3. Hong, S. W.; Huh, J.; Gu, X.; Lee, D. H.; Jo, W. H.; Park, S.; Xu, T.; Russell, T. P., *Proc. Natl. Acad. Sci. USA* **2012**, *109*(5), 1402-1406.
4. Park, S.; Lee, D. H.; Xu, J.; Kim, B.; Hong, S. W.; Jeong, U.; Xu, T.; Russell, T. P., *Science* **2009**, *323*, 1030-1033.
5. Al-Badril, Z. M.; Maddikeril, R. R.; Zha, Y.; Thaker, H. D.; Dobriyal, P.; Shunmugam, R.; Russell, T. P.; Tew, G. N., *Nature Comm.* **2011**, *2*, 486.

Honors and Awards

2016 ACS Award in Applied Polymer Science, 2008 National Academy of Engineering, 2004 APS Polymer Physics Prize, 2004 Dutch Polymer Award, 2003 ACS Cooperative Research Award in Polymer Science and Engineering

The Magic of Polypnictogen Compounds

Abstract

Organometallic polypnictogen compounds are an important class of compounds, valuable for many applications. Our interest is dedicated to pnictogen-rich organometallics, which usually can be synthesized from the E4 allotropes (E = P, As). Therefore, we have developed special approaches for the activation of the E4 molecules. In addition, we created novel E4-transfer reagents to avoid the handling hazardous starting materials. The talk will give an overview about the latest developments in this area and the stage of the use of the transfer reagents in main group and transition metal chemistry.

Prof. Manfred Scheer

Institute of Inorganic Chemistry, University of Regensburg

1980 Diploma Sc., University of Halle,
1983 Ph. D., University of Halle,
1996-2004 Associate-Professor of Chemistry at the Institute of Inorganic Chemistry of the University of Karlsruhe
2004- Full-Professor of Chemistry of the University of Regensburg
Web: http://www.ur.de/chemistry-pharmacy/inorganic-chemistry-scheer

Selected Publications

1. Schwarzmaier, C.; Sierka, M.; Scheer, M. *Angew. Chem. Int. Ed.* **2013**, *52*, 858.
2. Heinl, S.; Peresypkina, E.; Timoshkin, A. Y.; Mastrorilli, P.; Gallo, V.; Scheer, M. *Angew. Chem. Int. Ed.* **2013**, *52*, 10887.
3. Spitzer, F.; Grassl, Ch.; Balázs, G.; Zolnhofer, E. M.; Meyer, K.; Scheer, M. *Angew. Chem. Int. Ed.* **2016**, *55*, 4340.

Honors and Awards

2015 Member of the European Academy of Sciences and Arts, 2006 Searle Scholar; 2013 Wilhelm-Klemm-Award of the German Chemical Society; 2012 Elected member of the DFG Review Board on molecular chemistry; 2010 Associate Editor of “Chemical Communications”.

Metabolomics by NMR: a potential revolution in diagnosis

Abstract

Nuclear magnetic resonance (NMR) provides a quick and very reproducible method to obtain metabolic profiles of body fluids such as blood, urine, saliva etc. Several tens of metabolites can be easily identified and quantified in these fluids by NMR. Even the NMR spectrum as such immediately provides a very informative metabolic "fingerprint". Such fingerprint is specific for each individual and stable with time, unless a disease occurs. Many different diseases alter the fingerprint in specific ways. For some diseases the alteration occurs very early, and can even precede clinical symptoms. Using the NMR fingerprint as a diagnostic tool can potentially revolutionize preventive medicine, and healthcare in general.

Prof. Claudio Luchinat

Center of Magnetic Resonance, University of Florence, Florence, Italy

1976-1978 Post-doc, University of Florence

1978-1981 recipient of a CNR research grant, University of Florence

1981-1986 tenure researcher, University of Florence (Faculty of Pharmacy and Faculty of Sciences)

1986-1996 full professor of General and Inorganic Chemistry, Faculty of Agricultural Sciences, University of Bologna

1996- University of Florence

Selected Publications

1. Rammohan, N.; MacRenaris, K. W.; Moore, L., *et. al.*, *Nano Letters* Doi: 10.1021/acs.nanolett.6b03378: 2016.
2. Carlon, A.; Ravera, E.; Hennig, J., *et. al.*, *J.Am.Chem.Soc.* **2016,** *138*, 1601-1610.
3. Ravera, E.; Ciambellotti, S.; Cerofolini, L., *et. al.*, *Angew.Chem.Int.Ed.* **2016,** *55*, 1-5.
4. Benda, L.; Mareš, J.; Ravera, E., *et. al.*, *Angew.Chem.Int.Ed.* **2016,** *55,* 14713-14717.
5. Rotz, M. W.; Culver, K. S. B.; Parigi, G., *et. al.*, *ACS nano* **2015,** *9*, 3385-3396.

Honors and Awards

Recipient of the "Raffaello Nasini" gold medal award for Inorganic Chemistry of the Italian Chemical Society, 1989. Recipient of the Federchimica Award "For an Intelligent Future", 1994. Recipient of the 1996 European Medal for Biological Inorganic Chemistry, awarded by the Society of Biological Inorganic Chemistry. Recipient of the 2001 "GDRM gold medal for magnetic resonance". Co-founder of CERM and CIRMMP, of the spin-off ProtEra, of the no-profit research organization Fiorgen and of the spin-off Giotto Biotech S.r.l.

From imaging atoms to understanding human disease

Abstract

In 1986 Gerd Binnig and Heine Rohrer won the Physics Nobel prize for the invention of the scanning tunnelling microscope. Remarkably this was after only a few years since the first images of atoms were recorded. Although we did not know it at the time this invention and its developments effectively defined nanoscience; the understanding of matter at the nanoscale. Today, the window on the world that the tunnelling and force microscopes provided has blossomed into a world wide effort in nanoscience and nanotechnology with applications from fundamental science to commercial successes. The great opportunities in the next years will be the application of nanoscience into the diagnosis and treatment of human disease. In this lecture I will describe some of the earliest developments of the scanning tunnelling and atomic force microscopes and, jumping forward 30 years, demonstrate how these techniques can give a unique insight into the pathology of diseases such as Alzheimer's.

Prof. Sir Mark Welland

Nanoscience Centre, University of Cambridge, UK
1979 B.Sc., physics, University of Leeds
1984 Ph.D., physics, University of Bristol
1988 M.A., University of Cambridge
1985-1986 world trade visiting scientist at IBM Research Division in USA
1987- University of Cambridge
2003- the Nanoscience Centre at the University of Cambridge
2002- director of the Interdisciplinary Research Collaboration (IRC) in nanotechnology

Selected Publications

1. Cowburn, R. P.; Koltsov, D. K.; Adeyeye, A. O.; Welland, M. E.; Tricker, D. M., *Phys. Rev. Lett.* **1999**, *83* (5), 1042-1045.
2. Cowburn, R. P.; Welland, M. E., *Science* **2000**, *287* (5457), 1466-1468.
3. Knowles, T. P.; Fitzpatrick, A. W.; Meehan, S.; Mott, H. R.; Vendruscolo, M.; Dobson, C. M.; Welland, M. E., *Science* **2007**, *318* (5858), 1900-1903.
4. Knowles, T. P. J.; Waudby, C. A.; Devlin, G. L.; Cohen, S. I. A.; Aguzzi, A.; Vendruscolo, M.; Terentjev, E. M.; Welland, M. E.; Dobson, C. M., *Science* **2009**, *326* (5959), 1533-1537.
5. Smith, J. F.; Knowles, T. P. J.; Dobson, C. M.; MacPhee, C. E.; Welland, M. E., *Proc. Natl. Acad. Sci. USA* **2006**, *103* (43), 15806-15811.

Honors and Awards

From April 2008 until May 2012, Sir Mark was Chief Scientific Adviser to the UK Government Ministry of Defence. He was elected a Fellow of the Royal Society, a Fellow of the Royal Academy of Engineering, and a Fellow of the Institute of Physics in 2002, a Foreign Fellow of the National Academy of Sciences of India in 2008, and a Foreign Fellow of the Danish Academy of Sciences in 2010. Sir Mark was awarded a Knighthood in the Queen's Birthday Honours list in 2011.

Photochemical Upconversion and New Frontiers in Triplet Sensitization

Abstract

One focus of our research program involves the study of sensitized triplet fusion (TF) processes that convert low energy photons to higher energy light. Selective excitation of long-wavelength absorbing triplet sensitizers in the presence of appropriate molecular acceptors enables TF, resulting in either frequency upconverted light or the formation of desired chemical products. Various combinations of donor and acceptor have been explored and data will be presented on a number of these compositions spanning light conversions ranging from the near-UV to the near-IR. This presentation will also describe recent examples of upconversion phenomena realized in solid-state and fluidic polymeric materials along with emerging classes of sensitizers and acceptor/annihilator chromophores. Semiconductor (SC) nanocrystals are demonstrated to sensitize interfacial triplet-triplet energy transfer with molecular acceptors, providing a general paradigm for extracting triplet exciton energy from SC nanomaterials while extending their reactivity time by six orders-of-magnitude. The concept of SC nanocrystals serving as effective surrogates for molecular triplets suggests myriad of possible chemical and redox transformations relevant for fields as diverse as optoelectronics, solar energy conversion, and photobiology.

Prof. Felix N. Castellano

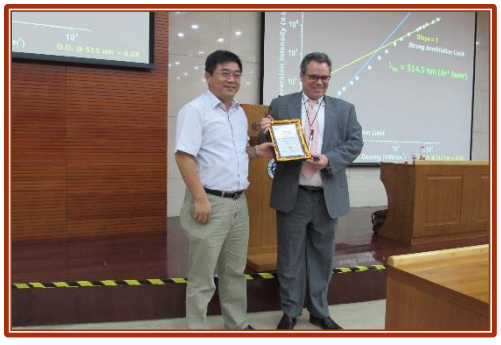
Department of Chemistry, North Carolina State University, USA
1991 B.A. Clark University, Chemistry, Research Advisor: Prof. F.T. Greenaway
1993 M.A. Johns Hopkins University, Chemistry, Research Advisor: Prof. G.J. Meyer
1996 Ph.D. Johns Hopkins University, Chemistry, Research Advisor: Prof. G.J. Meyer
1996 Postdoctoral Associate, Center for Fluorescence Spectroscopy, University of Maryland School of Medicine, Research Advisor: Prof. J.R. Lakowicz
1998-2013 Principal Member, Center for Photochemical Sciences, Bowling Green State University

Selected Publications

1. Castellano, F.N., *Inorg. Chem.* **2016**, *55*, 12483.
2. Younts, R.; Duan, H-S.; Gautam, B.; Saparov, B; Castellano, F.N.; Mitzi, D.; Gundogdu, K., *Adv. Mater.* **2016**, in press.
3. Mongin, C.; Golden, J.H.; Castellano, F.N., *ACS Appl. Mater. Interfaces* **2016**, *8*, 24038.
4. Garakyaraghi, S.; Crapps, P. D.; McCusker, C. E.; Castellano, F. N., *Inorg. Chem.* **2016**, *55*, 10628.
5. Khnayzer, R.S.; Olaiya, B.S.; El Roz, K.A.; Castellano, F.N., *ChemPlusChem* **2016**, *81*, 1090.

Honors and Awards

2005 BGSU Olscamp Research Award; 2002 BGSU Outstanding Young Scholar Award; 2002 Roseman Lecturer, Johns Hopkins University; 2002-2007 NSF CAREER Award; 1997-1998 NIH Postdoctoral Fellow.



Interactome disassembly during apoptosis occurs independent of caspase cleavage

Abstract

Protein-protein interaction networks (a.k.a. interactomes) define the functionality of all biological systems. In apoptosis, proteolysis by caspases is thought to initiate disassembly of protein complexes and cell death. Here we explore global changes in cytoplasmic and mitochondrial interactomes in response to Fas-mediated apoptosis to identify 17,991 interactions among 2,779 proteins, comprising the largest dynamic interactome to date. The majority of interactions were unaffected early in apoptosis but multiple complexes containing known caspase targets were disassembled. Nonetheless, proteome-wide analysis of proteolytic processing revealed little correlation between proteolytic and interactome changes. Our findings show that, in apoptosis, significant interactome alterations occur before and independently of caspase activity. Thus, apoptosis begins with a tight program of complex disassembly, leading to deactivation of relatively few, but key, protein complexes. This is followed by irreversible cleavage of these protein partners, locking the cell into an irreversible descent to cell death.

Prof. Leonard J. Foster

Department of Biochemistry and Molecular Biology, University of British Columbia, Canada

1996-2001 Doctoral candidate, Programme in Cell Biology, Hospital for Sick Children, Vancouver, Canada

2000-2004 Assistant Research Prof., Centre for Experimental BioInformatics, University of Southern Denmark

2005-2015 Assistant & Associate Professor, Biochemistry & Molecular Biology, University of British Columbia

2013-2015 Director, Centre for High-Throughput Biology, University of British Columbia

2015- Associate Director, Michael Smith Laboratories, University of British Columbia

2015- Professor, Biochemistry & Molecular Biology, University of British Columbia

Selected Publications

1. Foster, L. J.; de Hoog, C. L.; Zhang, Y. L., *et al.*, *Cell* **2006**, *125* (1), 187.
2. Karunakaran, K. P.; Yu, H.; Jiang, X., *et al.*, *Vaccine* **2015**, *33* (18), 2159.
3. Kristensen, A. R.; Gsponer, J.; Foster, L. J., *Nat. Methods* **2012**, *9* (9), 907.
4. Scott, N. E.; Brown, L. M.; Kristensen, A. R., *et al.*, *J. Proteomics* **2015**, *118,* 112.
5. Yu, H.; Karunakaran, K. P.; Kelly, I., *et al.*, *J. Immunol.* **2011**, *186* (6), 3615.

Honors and Awards

1996-2001 Doctoral Studentship, Visiting Lecturer Medical Research Council of Canada; 2002-2003 European Molecular Biology Organization Research Award; 2007-2008 Peter Wall Institute for Advanced Studies Early Career Scholar; 2009 Early Career Faculty Research Award, Faculty of Medicine, UBC; 2005-2010 Michael Smith Foundation for Health Research Award; 2005-2015 Canada Research Chair in Quantitative Proteomics; 2016 Killam Faculty Research Prize.

DNA Nanotechnology: From Basic Principles to Applications

Abstract

The base sequence in nucleic acids encodes substantial structural and functional information into the biopolymer. The lecture will address recent advances related to DNA nanostructures and will discuss the transitions of basic science to applications in the area of DNA nanotechnology. Specific topics that will be presented include: (i) The development of DNA machines and switches and their use to develop switchable catalytic processes, organize nanoparticles and control plasmonic properties; (ii) The development of nucleoapzymes as a new class of catalysts; (iii) Development of amplified sensing platforms, and particularly, DNA/nanomaterial-based sensors; (iv) The development of stimuli-responsive nano- and micro-carriers (mesoporous SiO_2 or microcapsules) for controlled drug delivery; (v) The synthesis of stimuli-responsive hydrogels and their application for controlled drug release, shape-memory matrices, and the design of surfaces exhibiting switchable catalytic, rigidity and interfacial electron transfer properties.

Prof. Itamar Willner

Institute of Chemistry, The Hebrew University of Jerusalem, Israel
1974-1978 Ph.D. Thesis, Physical Organic Chemistry, The Hebrew University of Jerusalem
1978-1980 Post-doctoral fellow, U.C. Berkeley, Physical Chemistry
1980-1981 Staff Scientist and Adjunct Assistant Professor, U.C. Berkeley
1981-1983 Senior Lecturer, Hebrew University of Jerusalem
1983-1986 Associate Professor, Hebrew University of Jerusalem
1986- Professor, Hebrew University of Jerusalem
Web: http://chem.ch.huji.ac.il/willner/

Selected Publications

1. Chandaluri, C.G.; Pelossof, G.; Tel-Vered, R.; Shenhar, R.; Willner, I., *ACS Appl. Mater. Interfaces* **2016**, *8*, 1440.
2. Aleman Garcia, M.A.; Hu, Y.; Willner, I., *Chem. Commun.* **2016**, *52*, 2153.
3. Golub, E.; Albada, H.B.; Liao, W.-C.; Willner, I., *J. Am. Chem. Soc.* **2016**, *138*, 164.
4. Lu, C.-H., Cecconello, A.; Qi, X.-J.; Wu, N.; Jester, S.S.; Famulok, M.; Matthies, M.; Schmidt, T. L.; Willner, I., *Nano Lett.* **2015**, *15*, 7133.
5. Kahn, J. S.; Trifonov, A.; Cecconello, A.; Guo, W.; Fan, C.; Willner, I., *Nano Lett.* **2015**, *15*, 7773.

Honors and Awards

2002 Israel Prize in Chemistry; 2002 Member of The Israel Academy of Sciences; 2004 Member of the European Academy of Sciences and Arts; 2008 Rothschild Prize in Chemistry; 2008 EMET Prize in Chemistry (under the auspices of the Prime Minister of Israel); 2009 Member of the German National Academy of Sciences Leopoldina.

Cancer Immune Therapy Targeting the Tumor Glycocalyx

Abstract

Successful tumors are able to evade the immune system, which is otherwise capable of killing transformed cells. Therapies that prevent this evasion have become revolutionary treatments for incurable cancers. This presentation will focus on our recent work targeting immune suppressive Siglec receptors and their sialylated glycan ligands, which are abundant within the cancer glycocalyx. We found that Siglec-ligand interactions can confer resistance to antibody-dependent cell cytotoxicity mediated by monoclonal antibody cancer drugs such as Herceptin. Based on this, we designed biotherapeutic molecules termed antibody-enzyme conjugates that selectively remove sialic acids from tumor cells and render them susceptible to immune cell killing. Editing the cancer cell glycocalyx with antibody-enzyme conjugates represents a new approach to cancer immune therapy.

Prof. Carolyn Bertozzi

Department of Chemistry, Stanford University

1988 BS, Harvard University,
1993 Ph. D., UC Berkeley,
1993-1996 Postdoc UCSF,
1996-2015 Assistant, Associate and Full Professor of Chemistry, UC Berkeley
2015- Anne T. and Robert M. Bass Professor of Chemistry, Stanford University
Web: http://web.stanford.edu/group/bertozzilab/index.html

Selected Publications

1. Schwarzmaier, C.; Sierka, M.; Scheer, M., *Angew. Chem. Int. Ed.* **2013**, *52*, 858.
2. Heinl, S.; Peresypkina, E.; Timoshkin, A. Y.; Mastrorilli, P.; Gallo, V.; Scheer, M., *Angew. Chem. Int. Ed.* **2013**, *52*, 10887.
3. Spitzer, F.; Grassl, Ch.; Balázs, G.; Zolnhofer, E. M.; Meyer, K.; Scheer, M., *Angew. Chem. Int. Ed.* **2016**, *55*, 4340.

Honors and Awards

Prof. Bertozzi is an elected member of the National Academy of Sciences, the American Academy of Arts and Sciences, and the German Academy of Sciences Leopoldina. Some awards of note include ACS Cope award (2017), the Lemelson-MIT award for inventors, Whistler Award, Ernst Schering Prize, MacArthur Foundation Fellowship, the ACS Award in Pure Chemistry, Tetrahedron Young Investigator Award, and Irving Sigal Young Investigator Award of the Protein Society. Her efforts in undergraduate education have earned her the UC Berkeley Distinguished Teaching Award and the Donald Sterling Noyce Prize for Excellence in Undergraduate Teaching.

Protein Analogous Micelles: Versatile, Modular Nanoparticles

Abstract

Peptides are functional modules of protein macromolecules that can be displayed apart from the whole protein to create biofunctional surfaces and interfaces, or can be re-assembled in new ways to create synthetic mimics of protein structures. Each of these routes are being employed to gain new insight into protein folding and to develop new, functional, biomolecular materials. Examples of work from our laboratory in this area using peptide-lipid conjugate molecules (peptide amphiphiles) will be discussed relating to multi-functional surfaces, DNA-binding peptide assemblies, and protein analogous micelles for cancer and cardiovascular therapeutics.

Prof. Matthew Tirrell

Founding Pritzker Director of the Institute for Molecular Engineering at the University of Chicago, Deputy Laboratory Director for Science at the Argonne National Laboratory
1973 B.S., Northwestern University,
1977 Ph. D., University of Massachusetts,
1977-1999 University of Minnesota
1999-2009 Dean of Engineering, University of California, Santa Barbara
2009-2011 Arnold and Barbara Silverman Professor and Chair of Bioengineering at the University of California, Berkeley
2011- Founding Pritzker Director of the Institute for Molecular Engineering at the University of Chicago, Deputy Laboratory Director for Science at the Argonne National Laboratory University of Chicago

Selected Publications

1. Brettmann, B. K.; Laugel, N.; Hoffmann, N., *et al.*, *J. Poly. Sci. Part a-Polymer Chemistry* **2016,** *54* (2), 284-291.
2. Farina, R.; Laugel, N.; Yu, J., *et al.*, *J. Phys. Chem. C* **2015,** *119* (26), 14805-14814.
3. Priftis, D.; Leon, L.; Song, Z., *et al.*, *Angew. Chem. Int. Edit.* **2015,** *54* (38), 11128-11132.
4. Yu, J.; Mao, J.; Yuan, G., *et al.*, *Polymer* **2016,** *98*, 448-453.
5. Yu, J.; Mao, J.; Yuan, G., *et al.*, *Macromolecules* **2016,** *49* (15), 5609-5617.

Honors and Awards

Professor Tirrell is a member of the National Academy of Engineering, the American Academy of Arts & Sciences and the Indian National Academy of Engineering, and is a Fellow of: the American Institute of Medical and Biological Engineers, the AAAS, and the APS.

Probing the 3D structures by transmission electron microscopy and electron diffraction - from zeolites and MOFs to proteins

Abstract

One of her main research interests is method development for accurate atomic structure determination of nano-sized crystals by electron crystallography. Her group has solved a number of complex structures of zeolites and mesoporous crystals by transmission electron microscopy. She is also working on synthesis, structure determination, topology analysis and applications of inorganic open-framework materials and metal-organic frameworks. In 2006, she received 100 MSEK from VR and VINNOVA to build up the Berzelii Center EXSELENT on Porous Materials and was the director 2006-2012. She has > 230 publications and four patents. Her group developed 9 software for quantitative analysis of high-resolution electron microscopy images and electron diffraction patterns. The software has been commecialized and used by > 200 laboratories.

Prof. Xiaodong Zou（邹晓冬）

Inorganic and Structural Chemistry Unit and deputy head of the Department of Materials and Environmental Chemistry, 1984 B.Sc., Peking University
1986 M.A., Beijing University of Technology, superviser: Prof. K.H. Kuo
1995 Ph.D., Stockholm University, structural chemistry
1995 postdoc., Lund University, advisor: Prof. David R. Veblen
1996- faculty of Stockholm University
2005- professor, Stockholm University

Selected Publications

1. Inge, A. K.; Christensen, K. E.; Willhammar, T., *et al.*, *Crystal Growth & Designs* **2016,** *16* (12), 6967-6973.
2. Tang, L. Q.; Shi, L.; Bonneau, C., *et al.*, *Nat. Mater.* **2008,** *7* (5), 381-385.
3. Willhammar, T.; Sun, J. L.; Wan, W., *et al.*, *Nat. Chem.* **2012,** *4* (3), 188-194.
4. Zou, X. D.; Conradsson, T.; Klingstedt, M., *et al.*, *Nature* **2005,** *437* (7059), 716-719.

Honors and Awards

sShe received several awards including Tage Erlander Prize for Science and Technology 2002 and Göran Gustafsson Prize in Chemistry 2008, both given by the Royal Swedish Academy of Sciences, the K.H. Kuo Award for Distinguished Scientist 2010 and the Arrhenius medal 2012 given by the Swedish Chemical Society. She is the fellow of the Royal Chemical Society (FRCS), the council member of the International Zeolite Association and the member of Structure Commission of International Zeolite Association.

北京大学研究生教育的再思考

Abstract

林建华校长深度思考全球化时代背景下的北大研究生教育，总结过去，展望未来，守正创新，将北大学术研究和研究生教育事业推向新的高峰。吹响号角再出发，将北大建设成为一所伟大的学校！

Prof. Jianhua Lin (林建华)

College of Chemistry and Molecular Engineering, Peking University
1982 B.Sc., Peking University
1986 Ph. D., Peking University
1988-1990 Research Scientist, Max-Plank Institute of Solid State Research, Stuttgart, Germany
1990-1993 Post Doctoral Fellow, Department of Chemistry, Iowa State University, US
1986- faculty of Peking University

Selected Publications s

1. Sun, J. L.; Yang, M.; Li, G. B.; Yang, T.; Liao, F. H.; Wang, Y. X.; Xiong, M.; Lin, J. H., *Inorg. Chem.* **2006**, *45*(23), 9151.
2. Li, L. Y.; Li, G. B.; Wang, Y. X.; Liao, F. H.; Lin, J. H., *Inorg. Chem.* **2005**, *44*, 8243.
3. Li, Z. F.; Sun, J. L.; You, L. P.; Jiao, H.; Li, G. B.; Jing, X. P.; Liao, F. H.; Lin, J. H.; Lee, S., *Chem. Mater.* **2005**, *17*, 2186.
4. Lin, J. H.; Sheptyakov, D.; Wang, Y. X.; Allenspach, P.; *Chem. Mater.* **2004**, *16*, 2418.
5. Ju, J.; Lin, J. H.; Yang, T.; Li, G. B.; Liao, F. H.; Wang, Y. X.; You, L. P., *Chem. Eur. J.* **2004**, *10*, 3901.

Honors and Awards

1995 年获国家教委科学技术二等奖，1997 年获国家杰出青年基金资助，2009 年获国家级教学成果一等奖。

From ring polymer molecular dynamics to spin dynamics

Abstract

During the past ten years, most of the work in my group has been on the development and application of ring polymer molecular dynamics (RPMD). This is a simple theory which provides a practical way to include quantum mechanical (zero point energy and tunneling) effects in the nuclear motion in calculations of chemical reaction rates and in simulations of condensed phase systems. More recently, we have also begun to work on spin dynamics, with a particular interest in understanding the role of radical pair recombination reactions in the avian retina in providing the magnetic compass sense of migratory birds. In this lecture, I will review both of these topics, and then end by mentioning some related problems that we are currently working on.

Prof. David E. Manolopoulos

Physical and Theoretical Chemistry Laboratory, University of Oxford

1984 B.A. in Natural Sciences (First Class), University of Cambridge
1988 Ph.D. in Theoretical Chemistry, University of Cambridge
1990-1995 Lecturer in Physical Chemistry, University of Nottingham
1995-2005 Lecturer in Physical and Theoretical Chemistry, University of Oxford
2005- Professor of Theoretical Chemistry, University of Oxford
Web: http://research.chem.ox.ac.uk/david-manolopoulos.aspx

Selected Publications

1. Habershon, S.; Manolopoulos, D. E.; Markland T. E.; Miller, T. F., *Ann. Rev. Phys. Chem.* **2013**, *64*, 387.
2. Hiscock, H. G.; Worster, S.; Kattnig, D. R.; Steers, C.; Jin, Y.; Manolopoulos, D. E.; Mouritsen, H.; Hore, P. J., *Proc. Natl. Acad. Sci. USA* **2016**, *113*, 4634.

Honors and Awards

2013 Member of the International Academy of Quantum Molecular Science, 2011 Fellow of the Royal Society. 2000 Annual Prize of the International Academy of Quantum Molecular Science. Royal Society of Chemistry Medals: Marlow (1995), Corday-Morgan (1997), Chemical Dynamics (2009).

Heterogeneous Single-Atom Metal Catalysts for Efficient Fuel Processing and Green Chemicals Production

Abstract

Catalyst design and development aims at more efficient and sustainable chemical processes. To this end, identification of the active catalytic site and design of catalysts with 100% atom efficiency has been a long-standing goal in heterogeneous catalysis. A novel approach to reaching this goal through single-atom metal catalysts has emerged in the recent literature. Atomically dispersed supported metal catalysts offer new prospects for low-cost fuel processing and green chemicals production (*Annu. Rev. Chem. Biomol. Eng.* 2012, 3). In this presentation, metal catalysts stabilized as single atoms/cations on various supports will be reviewed drawing examples from a variety of reactions, including the low-temperature water-gas shift reactions (*Science* 2003, 301, 935; *Science* 2014, 346, 1498; *J. Am. Chem. Soc.* 2015, 137, 3470), methanol steam reforming, and methanol and ethanol dehydrogenation reactions; and several selective hydrogenation reactions (*Science* 2012, 335, 1209; *Nat. Commun.* 2015, 6, 8550). We will demonstrate how reaction mechanisms involving single metal atoms/cations, transcend support structure and composition as long as the metal atom-centered, oxygen bonded active site, M-Ox-, is allowed to form stably. A unique "signature" of the metal (Au, Pt, Pd, *etc.*) at the atomic state is preserved, distinct however from the corresponding extended metal catalyst. Novel synthesis methods will be discussed as will be the stability of atomically dispersed catalysts in various reaction environments.

Prof. Maria Flytzani-Stephanopoulos

Department of Chemical and Biological Engineering, Tufts University, Medford, MA, USA
B.S., Chemical Engineering, National Technical University of Athens, Greece
M.S., Chemical Engineering, University of Florida
Ph.D., Chemical Engineering, University of Minnesota
Web: http://ase.tufts.edu/nano-cel/

Selected Publications

1. Garbarino, G.; Wang, C.; Valsamakis, I., *et al.*, *Applied Catalysis B-Environmental* **2017**, *200*, 458-468.
2. Wang, C.; Garbarino, G.; Allard, L. F., et al., *ACS Catal.* **2016,** *6* (1), 210-218.
3. Shan, J.; Lucci, F. R.; Liu, J., et al., *Surf. Sci.* **2016,** *650*, 121-129.
4. Liu, J.; Lucci, F. R.; Yang, M., et al., *J. Am. Chem. Soc.* **2016,** *138* (20), 6396-6399.
5. Lucci, F. R.; Liu, J.; Marcinkowski, M. D., et al., *Nat. Commun.* **2015,** *6*.

Honors and Awards

2016 Carol Tyler Award, IPMI; 2015 Distinguished Professor; 2015 Graduate Teaching and Mentoring Award, School of Engineering, Tufts University; 2014 Member, National Academy of Engineering; 2014 Associate Editor, Science Advances; 2013 Director-at-Large, North American Catalysis Society; 2013 Giuseppe Parravano Memorial Award, The Michigan Catalysis Society; 2012 2nd Vice Chair, AIChE/Catalysis and Reaction Engineering Division

Research Diversity on Complex Hydride

Abstract

Complex hydrides with hydride complex(es) and metal cation(s) have been practically used as reducing agents for many chemical reactions. After the research series of the reversible decomposition and recombination reactions of the complex hydrides themselves, they became one of the candidates for hydrogen storage materials. Also, a new research direction was emerged triggered by the report of lithium super-ionic conductivity in the complex hydrides, and nowadays it is of importance to apply them to advanced battery devices. Furthermore, a recent topic on the highest critical-temperature superconductivity in the sulfur di-/tri-hydride system has stimulated rapidly growing interest in the exploration of hydrogen-richer complex hydrides. The presenter will review and forecast the complex hydride research.

Prof. Shin-ichi ORIMO

WPI Advanced Institute for Materials Research (WPI-AIMR) / Institute for Materials Research, Tohoku University

1995 Ph. D., Faculty of Integrated Arts and Sciences, Hiroshima University
1995~2002 Research Associate, Hiroshima University
1998~1999 Guest Researcher, Max-Planck Institute for Metal Research, as Humboldt Foundation Fellow and MEXT Fellow)
2002~2009 Associate Professor, Institute for Materials Research, Tohoku University
2009~ Professor, Head of the Section for Hydrogen Functional Materials
2012~2014 Special Advisor to the University President (~2014)
2013~ PI, WPI Advanced Institute for Materials Research (WPI-AIMR)
2015~ Chair, the 190th University-Industry Collaborative Committee
Web: http://www.hydrogen.imr.tohoku.ac.jp/

Selected Publications

1. S. Orimo, *et al.*, Chem. Rev. (Review Article) **2007**, *107*, 4111.
2. M. Matsuo, S. Orimo, *Adv. Energy Mater.* (Review Article) **2011**, *1*, 161.
3. A. Unemoto, M. Matsuo, S. Orimo, *Adv. Func. Mater.* (Feature Article) **2014**, *103*, 133903.
4. T. J. Udovic; M. Matsuo, W.S. Tang, S. Orimo *et al.*, *Adv. Mater.* **2014**, *26*, 7622.
5. S.takagi, Y. Iijima, T. Sato, S. Orimo *et al.*, *Angew. Chem. Int. Ed.* **2015**, *54*, 5650.

Honors and Awards

2011 Funding Program for Next Generation World-Leading Researchers (Cabinet Office, Council for Science and Technology Policy); 2011 Metals Meritorious Award (The Japanese Institute of Metals); 2012 Prize for Science and Technology (The Commendation for Science and Technology by the Minister, MEXT); 2015 International Hydrogen & Energy Award.

Metal-Catalyzed Cross-Couplings of Alkyl Electrophiles

Prof. Gregory C. Fu

Division of Chemistry and Chemical Engineering, California Institute of Technology, USA

1985 B.S., Chemistry, with Professor K. Barry Sharpless, Massachusetts Institute of Technology
1991 Ph.D., Chemistry, with Professor David A. Evans, Harvard University
1991–1993 Postdoctoral fellow with Professor Robert H. Grubbs, California Institute of Technology
1993–1998 Assistant Professor of Chemistry, Massachusetts Institute of Technology
1998–1999 Associate Professor of Chemistry, Massachusetts Institute of Technology
1999–2007 Professor of Chemistry, Massachusetts Institute of Technology
2007–2012 Firmenich Professor of Chemistry, Massachusetts Institute of Technology
2012–2016 Altair Professor of Chemistry, California Institute of Technology
2016–present Norman Chandler Professor of Chemistry, California Institute of Technology

Selected Publications

1. Kainz, Q. M.; Matier, C. M.; Bartoszewicz, A.; Zultanski, S. L.; Peters, J. C.; Fu, G. C., *Science* **2016**, *351*, 681–684.
2. Zuo, Z.; Cong, H.; Li, W.; Choi, J.; Fu, G. C.; MacMillan, D. W. C., *J. Am. Chem. Soc.* **2016**, *138*, 1832–1835.
3. Chu, C., K.; Liang, Y.; Fu, G. C., *J. Am. Chem. Soc.* **2016**, *138*, 6404–6407.
4. Johnson, M. W.; Hannoun, K. I.; Tan, Y.; Fu, G. C.; Peters, J. C., *Chem. Sci.* **2016**, *7*, 4091–4100.
5. Ziegler, D. T.; Fu, G. C., *J. Am. Chem. Soc.* **2016**, *138*, 12069–12072.

Honors and Awards

2015 Associated Students of the California Institute of Technology (ASCIT) Teaching Award, 2015 Yamada–Koga Prize 2014 Fellow, National Academy of Sciences, 2012 Award for Creative Work in Synthetic Organic Chemistry, American Chemical Society, 2007 Fellow, American Academy of Arts and Sciences, 2007 Catalysis Science Award, Mitsui Chemicals, 2006 Mukaiyama Award, Society of Synthetic Organic Chemistry of Japan, 2004 Elias J. Corey Award, American Chemical Society, 2001 Springer Award in Organometallic Chemistry, 2000 School of Science Undergraduate Teaching Prize, MIT, 2000 Chan Memorial Award in Organic Chemistry, 1998 Arthur C. Cope Scholar Award, American Chemical Society, 1997 Camille Dreyfus Teacher-Scholar Award, 1997 Alfred P. Sloan Research Fellow, 1996 Lilly Grantee Award, Eli Lilly, 1996 Cottrell Scholar Award, Research Corporation, 1994 National Science Foundation Young Investigator Award, 1993 Camille and Henry Dreyfus Foundation New Faculty Award

Supramolecular Nanosystems for Smart Diagnosis and Therapy of Intractable Diseases

Abstract

Nanomedicine has received progressive interest for the treatment of intractable diseases and non-invasive diagnosis. Nanosystems, which have several advantages including controlled drug release, tissue penetrating ability and reduced toxicity, play a key role in nanomedicine as drug carriers, gene vectors, and imaging probes. Polymeric micelles as platform nanosystems for molecular therapy is a promising choice for versatile drug incorporation.

Prof. Kazunori Kataoka

1) Innovation Center of NanoMedicine (iCONM), Kawasaki Institute of Industry Promotion Policy
2) Policy Alternatives Research Institute, the University of Tokyo

1974 B.Eng., The University of Tokyo
1979 Ph.D., The University of Tokyo
1994-1998 Full Professor, Department of Materials Engineering, Tokyo University of Science
1998-2016 Full Professor, Department of Materials Engineering, The University of Tokyo
2016- Full Professor, Policy Alternatives Research Institute, The University of Tokyo
Web: http://www.bioeng.t.u-tokyo.ac.jp/en/faculty/16_kataoka.html

Selected Publications

1. H. Cabral, K. Kataoka, *J. Control. Release* **2014**, *190,* 70-72.
2. H. Uchida, K. Itaka, S. Uchida, T. Ishii, T. Suma, K. Miyata, M. Oba, N. Nishiyama, K. Kataoka, *J. Am. Chem. Soc.* **2016**, *138*(5), 1478-1481.
3. P. Mi, D. Kokuryo, H. Cabral, H. Wu, Y. Terada, T. Saga, I. Aoki, N. Nishiyama, K. Kataoka, *Nature Nanotechnol.* **2016**, *11*(8), 724-730.

Honors and Awards

member of the Science Council of Japan (2006), the Founder's Award from the Controlled Release Society (2008), the National Institute of Materials Science Award, Japan (2009), Humboldt Research Award from Alexander von Humboldt Foundation (2012), SPSJ Award for Outstanding Achievements in Polymer Science and Technology (2014), Lifetime Achievement Award, Journal of Drug Targeting (2014).

Chemical Functionalization of Synthetic Carbon Allotropes

Abstract

Synthetic carbon allotropes (SCAs) such as fullerenes, carbon nanotubes and graphene are characterized by a number of outstanding and unprecedented properties such as electrical conductivity, mechanical stability and transparency. They are often regarded to be among the most promising candidates for future high performance materials. To reach this challenging goal, chemical functionalization of the parent systems will play a key role. Covalent and non-covalent transformations of SCA can considerably improve and tailor their solubility and processibility and combine their properties with those of other compound classes. For this purpose we are exploring the fundamental chemical properties of SCAs and determine, for example, reaction mechanisms, selectivities of transformations and characteristic addition patterns. Binding of a large variety of organic building blocks including dendrimers, porphyrines, rylenes, sugars and peptides has been accomplished. Using our knowledge in wet-chemical functionalization of fullerenes, carbon nanotubes and graphene; new molecular architectures with remarkable functions such as photo-induced electron transfer, superoxide dismutation and protein simulation have been created.

Prof. Andreas Hirsch

University of Erlangen-Nürnberg, Institute of Organic Chemistry II

1990 Ph. D., the University of Tübingen

1990-1991 Postdoctoral fellow at the Institute for Polymers and Organic Solids in Santa Barbara, California

1992-1994 A research associate at the Institute for Organic Chemistry in the University of Tübingen

1994 A Professor of Organic Chemistry in the Chemistry Faculty at the University of Karlsruhe

1995- Full Professor of Organic Chemistry at the Friedrich-Alexander-Universität Erlangen-Nuremberg

2000 Declined an offer for the Chair for Organic Chemistry at the University of St. Andrews, Scotland

2004 Adjunct Professor at Rice University in Houston

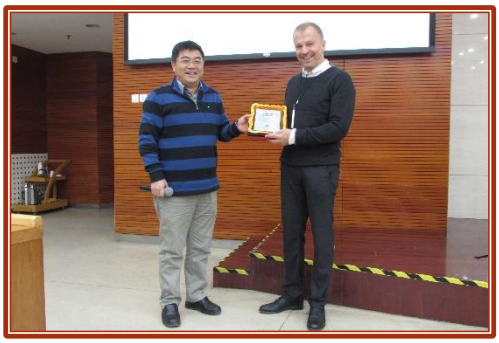
2004-2008 Fachkollegiat for Molecular Chemistry at the Deutsche Forschungsgemeinschaft DFG

2005 Declined an offer for a joint appointment as Welch Professor of Chemistry at Rice University Houston and Welch-Cullen Professor of Chemistry and Nanotechnology at University of Texas Health Science Center in Houston. The offer was initiated and strongly supported by Prof. Smalley (Nobel Prize in Chemistry 1996 for the discovery of the fullerenes).

2006 Visiting Professor at the University of Nikosia in Cyprus

2011 Visiting Professor at the University of Padova in Italy

Web: http://www.hirsch.chemie.uni-erlangen.de/en/welcome.html



Selected Publications

1. Ehli, C.; Oelsner, C.; Guldi, D. M., et. al., *Nature Chem.* **2009**, *1*, 243.
2. Hirsch, A. *Nature Mater.* **2010**, *9*, 868.
3. Englert, J. M.; Dotzer, C.; Yang, G., et. al., *Nature Chem.* **2011**, *3*, 279.
4. Schäfer, R. A.; Englert, J. M.; Wehrfritz, P., *et. al., Angew. Chem. Int. Ed.* **2013**, *52*, 754.
5. Schäfer, R. A; Dasler, D.; Mundloch, U., et. al., *J. Am. Chem. Soc.* **2016**, *138*, 1647.

Honors and Awards

The Otto-Röhm Research Award (1994), The ADUC Award für Habilitanden (1994), The Elhuyar-Goldschmidt-Prize of the Spanish and German Chemical Societies (2006), Professor of the Year (Unicum, Beruf, Germany) (2007), The First ERC Advanced Grant (GRAPHENOCHEM) of the FAU (2010), The Max Grundig Award (2012), The Medal of the Organic Institute of the Academy of Sciences of the Czech Republic (2012)

Modeling the Action of Complex Biological Systems on a Molecular Level

Abstract

Despite the enormous advances in structural studies of biological systems we are frequently left without a clear structure function correlation and cannot fully describe how different systems actually work. This introduces a major challenge for computer modeling approaches that are aimed at a realistic simulation of biological functions. The unresolved questions range from the elucidation of the basis for enzyme action to the understanding of the directional motion of complex molecular motors. Here we review the progress in simulating biological functions, starting with the early stages of the field and the development of QM/MM approaches for simulations of enzymatic reactions. We provide overwhelming support to the idea that enzyme catalysis is due to electrostatic preorganization and then move to the renormalization approaches aimed at modeling long time processes, demonstrating that dynamical effects cannot change the rate of the chemical steps in enzymes. Next we describe the use our electrostatic augmented coarse grained (CG) model and the renormalization method to simulate the action of different challenging complex systems. It is shown that our CG model produces, for the first time, realistic landscapes for vectorrial process such as the actions of F1 ATPase, F0 ATPase and myosinV. It is also shown that such machines are working by exploiting free energy gradients and cannot just use Brownian motions as the vectorial driving force. Significantly, at present, to the best of our knowledge, these studies are the only studies that reproduced consistently (rather than assumed) a structure based vectorial action of molecular motors. We also describe a breakthrough in CG modeling of voltage activated ion channels. We also outline a recent simulation of the tag of war between staled elongated peptide in the ribosome and the translocon as an illustration of the power of our CG approach. The emerging finding from all of our simulations is that electrostatic effects are the key to generating functional free energy landscapes. Finally, we present some thought on the future of the field, taking drug resistance as an example.

Prof. Arieh Warshel

University of Southern California

Education: BSc Chemistry (Technion, Israel), MSc and PhD Chemical Physics (Weizmann Institute of Sciences, Israel)
Role(s): Group leader, Dana and David Dornsife Chair in Chemistry & Distinguished Professor of Chemistry and Biochemistry at USC
Web: http://laetro.usc.edu/index.html

Selected Publications

1. Kim, I.; Warshel, A., *J. Phys. Chem. B* **2016**, *120* (3), 418-432.
2. Lameira, J.; Kupchencko, I.; Warshel, A., *J. Phys. Chem. B* **2016**, *120* (9), 2155-2164.
3. Mukherjee, S.; Bora, R. P.; Warshel, A., *Q. Rev. Biophys.* **2015**, *48* (4), 395-403.
4. Mukherjee, S.; Warshel, A., *Proc. Natl. Acad. Sci. U. S. A.* **2015**, *112* (46), 14121-14122.
5. Vorobyov, I.; Kim, I.; Chu, Z. T., *et al.*, *Proteins-Structure Function and Bioinformatics* **2016**, *84* (1), 92-117.

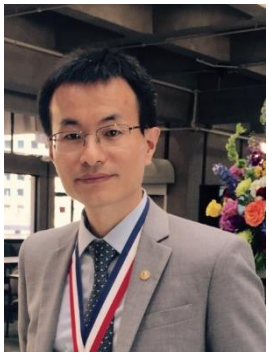
Honors and Awards

Nobel Laureate (Chemistry, 2013), Member National Academy of Sciences (2009), Honorary Fellow of the Royal Society of Chemistry (2008), Fellow of the Biophysical Society (2000)

CO_2 + H_2O + Sunlight → Chemical Fuels + O_2

Abstract

Solar-to-chemical (STC) production using a fully integrated system is an attractive goal, but to-date there has yet to be a system that can demonstrate the required efficiency, durability, or be manufactured at a reasonable cost. One can learn a great deal from the natural photosynthesis where the conversion of carbon dioxide and water to carbohydrates is routinely carried out at a highly coordinated system level. There are several key features worth mentioning in these systems: spatial and directional arrangement of the light-harvesting components, charge separation and transport, as well as the desired chemical conversion at catalytic sites in compartmentalized spaces. In order to design an efficient artificial photosynthetic materials system, at the level of the individual components: better catalysts need to be developed, new light-absorbing semiconductor materials will need to be discovered, architectures will need to be designed for effective capture and conversion of sunlight, and more importantly, processes need to be developed for the efficient coupling and integration of the components into a complete artificial photosynthetic system. In this talk I will begin by discussing the challenges associated with fixing CO_2 through traditional chemical catalytic means, contrasted with the advantages and strategies that biology employs through enzymatic catalysts to produce more complex molecules at higher selectivity and efficiency. I then discuss a number of different photosynthetic biohybrid systems (PBS) architectures from the last few years, and the numerous strategies to interface biotic and abiotic components. Each demonstrates the advantages of PBSs in converting sunlight, H_2O and CO_2 into food, fuels, pharmaceuticals, and materials. Finally, I will outline the future of this field, opportunities for improvement, and its role in sustainable living here on Earth, and beyond.



Prof. Peidong Yang

Department of Chemistry and Department of Materials Science Engineering, University of California, Berkeley

B. A. Chemistry, University of Science and Technology in China (1993); Ph. D. Chemistry, Harvard University (1997); Postdoctoral Fellow, University of California, Santa Barbara (1997-1999);
Web: http://nanowires.berkeley.edu/

Selected Publications

1. Kong, Q.; Kim, D.; Liu, C., *et al.*, *Nano Lett.* **2016,** *16* (9), 5675-5680.
2. Kornienko, N.; Sakimoto, K. K.; Herlihy, D. M., *et al.*, *Proc. Natl. Acad. Sci. U. S. A.* **2016,** *113* (42), 11750-11755.
3. Niu, Z.; Becknell, N.; Yu, Y., *et al.*, *Nat. Mater.* **2016,** *15* (11), 1188-1194.
4. Sakimoto, K. K.; Zhang, S. J.; Yang, P., *Nano Lett.* **2016,** *16* (9), 5883-5887.
5. Zhang, D.; Yu, Y.; Bekenstein, Y., *et al.*, *J. Am. Chem. Soc.* **2016,** *138* (40), 13155-13158.

Honors and Awards

Camille and Henry Dreyfus New Faculty Award (1999); 3M Untenured Faculty Award (2000). Research Innovation Award (2001); Alfred P. Sloan Fellow (2001); NSF CAREER Award (2001); Hellman Family Faculty Award (2001); ACS ExxonMobil Solid State Chemistry Award (2001); Beckman Young Investigator Award (2002). MIT Tech. Review TR 100 (2003); ChevronTexaco Chair in Chemistry, Berkeley (2003); First Chairperson for American Chemical Society, Nanoscience subdivision (2003); Camille Dreyfus Teacher-Scholar Award (2004); Dupont Young Professor Award (2004), Julius Springer Prize for Applied Physics (2004), MRS Outstanding Young Investigator Award (2004), ACS Pure Chemistry Award (2005), University of Wisconsin McElvain Lectureship (2006), Chinese Academy of Science Molecular Science Forum Lectureship (2006), NSF A. T. Waterman Award (2007), Scientific American 50 Award (2008).

How to make well-defined silicone materials: Recent new synthetic methods

Abstract

Silicon compounds, especially silicones and silsesquioxanes are now widely used in our life, and recent demand for high-function materials drastically push up the research on these compounds to high level. In this presentation, I will summarize our research in the last two decades, and introduce the synthetic methods, properties, reactions, and applications of various silicon compounds. In addition, I will introduce several unique silicon compounds including reactive species (octasilacubanes) or those with interesting structures while indicating how to build up research career.

Prof. Masafumi Unno

Department of Chemistry and Chemical Biology and International Education and Research Center for Silicon Science, Faculty of Science and Technology, Gunma University

1988 Ph.D. The University of Tokyo (Profs. Inamoto and Okazaki)
1992.5–1993.1 Frontier Researcher, PDC, RIKEN (Prof. M. Kira)
1993.1–2002.3 Assistant Professor, Gunma University
2002.4–2005.3 Associate Professor, Gunma University
2005.4–present Professor, Gunma University
2009.8–present Director of Silicon Center, Gunma University

Web: http://element.chem-bio.st.gunma-u.ac.jp/index-e.html

Selected Publications

1. Unno, M.; Suto, A.; Matsumoto, T., *Russian Chemical Reviews* **2013,** *82* (4), 289-302.
2. M. Unno and H. Matsumoto, "Reactions of Octasilacubane", in *Organosilicon Chemistry VI，Eds. N. Auner and J. Weis, WILEY-VCH Verlag, Weinheim,* **2005**, pp. 373–380.
3. Endo, H.; Takeda, N.; Takanashi, M., et al., *Silicon* **2015,** *7* (2), 127-132.
4. Murakami, S.; Egawa, Y.; Kuramochi, C., et al., *Chem. Lett.* **2016,** *45* (3), 309-311.
5. Oguri, N.; Takeda, N.; Unno, M., *Chem. Lett.* **2015,** *44* (11), 1506-1508.

Honors and Awards

1999.11 Incentive Award, The Society of Silicon Chemistry, Japan
2004. 2 The 7th Yokoyama Scientific Research Award

Functional Glycomics Through Chemical Synthesis

Abstract

Most eukaryotic cell surface and secreted proteins are modified by covalently-linked glycans which are essential mediators of biological processes such as protein folding, cell signaling, fertilization, embryogenesis, and the proliferation of cells and their organization into specific tissues. Overwhelming data supports the relevance of glycosylation in pathogen recognition, inflammation, innate immune responses, the development of autoimmune diseases, and cancer. Two research topics will be discussed. The first topic deals with the development of a carbohydrate-based cancer vaccine in which several immuno-modulatory activities are captures in a relatively small synthetic compound. We have shown that an appropriately glycosylated MUC1 peptide covalently linked to a promiscuous helper T-epitope and a Toll-like receptor (TLR) agonist can elicit robust humoral and cellular immune responses and was efficacious in reversing tolerance and generating a therapeutic response in a mouse model of mammary cancer. The second topic demonstrates that the complex architecture of N-glycans is critical for mediating biological functions. This was discovered by the developed a chemo-enzymatic methodology that makes it possible to prepare libraries of highly complex asymmetrically substituted glycans. The power of the methodology was demonstrated by the preparation of a tri-antennary oligosaccharide that can inhibit binding of spermatozoan to the zona pellucida of human oocytes. Furthermore, we have prepared a series of complex oligosaccharides that were printed as microarrays and screened for binding to lectins and influenza-virus hemagglutinins, which demonstrated that recognition is modulated by presentation of minimal epitopes in the context of complex N-glycans.

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2013-present UGA Foundation Distinguished Professor in Biochemical Sciences, Franklin College of Arts and Sciences, University of Georgia
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Selected Publications

1. Friscourt, F.; Ledin, P.A.; Mbua, N.E., *et. al., J. Am. Chem. Soc.* **2012**, *134*, 5381.
2. Wang, Z.; Chinoy, Z.; Ambre, S., *et. al., Science*. **2013**, *341*, 379.
3. Sun, T.; Yu, S.H.; Zhao, P., *et. al., J. Am. Chem. Soc.* **2016**, *138*, 11575.

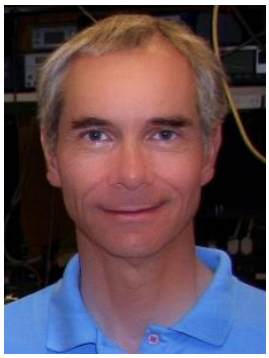
Honors and Awards

2016 Cope Mid Career Scholar Award from the American Chemical Society; 2015 Claude S. Hudson Award by the Division of Carbohydrate Chemistry, ACS; 2014 Roy L. Whistler International Award in Carbohydrate Chemistry, International Carbohydrate Organization; 2004 Horace Isbell Award by the Division of Carbohydrate Chemistry, ACS.

Protein dynamics: from computer, to test tube, to the cell

Abstract

Much progress has been made in bringing together computation and experiment to describe protein folding. I will discuss some of the breakthroughs that have allowed complete folding of a protein to be simulated on a computer, including all atoms with full solvent, and how the results compare with experimental measurements of fast protein kinetics. The next challenge is to understand how cells modulate the folding and interaction of proteins, and I will discuss new experiments to look at proteins inside cells, using temperature and osmotic jumps to stress cells and observe protein dynamics. Evolution is likely to act on weakly coupled networks of proteins that remain intact only inside cells, not just on the obvious strong protein-protein interactions that have been studied in the past.



Prof. Martin Gruebele

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1984 B.S. Chemistry, University of California at Berkeley
1988 Ph. D., Chemistry, University of California at Berkeley
1989-1992 Postdoctoral Fellow, Caltech (with Ahmed Zewail)
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2008- James R. Eiszner Chair in Chemistry, Professor of Physics, Professor in CBQB
1998-2005 Senior editor, Journal of Physical Chemistry
2013-present Associate Editor, JACS
Web: http://www.scs.illinois.edu/~mgweb

Selected Publications

1. Ebbinghaus, S.; Dhar, A.; McDonald, D., et al., *Nat. Methods* **2010,** *7* (4), 319-323.
2. Yang, W. Y.; Gruebele, M., *Nature* **2003,** *423* (6936), 193-197.
3. Gruebele, M., *C. R. Biol.* **2005,** *328* (8), 701-712.

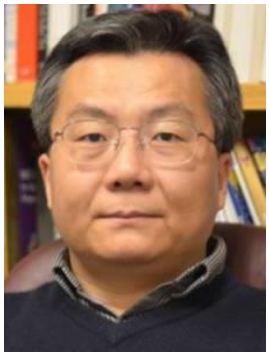
Honors and Awards

ACS National Award: Nakanishi Prize (ACS, 2016)
Member, National Academy of Sciences (USA, 2013)
Fellow of the American Academy of Arts and Sciences (USA, 2010)
Raymond and Beverly Sackler International Prize (Israel, 2008)
Member, German National Academy of Science (Leopoldina) (Germany, 2008)

Tuning Nanoparticle Catalysis for Efficient Electrochemical Reactions

Abstract

Recent advance in solution phase chemical reactions has made it possible to design and synthesize nanoparticles with nearly precise controls on nanoparticle sizes, shapes, compositions and structures for catalytic applications. In this talk, I will summarize the common methods we used to synthesize monodisperse nanoparticles, especially intermetallic nanoparticles, core/shell nanoparticles, nanowires and their self-assemblies on conducting supports. I will use Au-, Pt-, Pd-, Fe-, and Cu-based elemental and alloy nanoparticles as examples to demonstrate the rational tuning and enhancement of nanoparticle catalysis for electrochemical reduction of O_2, electrochemical oxidation of HCOOH and other chemical reactions for renewable energy applications.



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Selected Publications

1. Guo, S.; Zhang, X.; Zhu, W., et al., *J. Am. Chem. Soc.* **2014,** *136* (42), 15026-15033.
2. Li, Q.; Wu, L.; Wu, G., et al., *Nano Lett.* **2015,** *15* (4), 2468-2473.
3. Mendoza-Garcia, A.; Zhu, H.; Yu, Y., et al., *Angew. Chem. Int. Edit.* **2015,** *54* (33), 9642-9645.
4. Wu, L.; Li, Q.; Wu, C. H., et al., *J. Am. Chem. Soc.* **2015,** *137* (22), 7071-7074.
5. Zhu, W.; Zhang, Y.-J.; Zhang, H., et al., *J. Am. Chem. Soc.* **2014,** *136* (46), 16132-16135.

Honors and Awards

孙教授现在是布朗大学分子和纳米创新研究所副主任，英国皇家化学会期刊 Nanoscale 的副主编及英国皇家化学学会 Fellow。先后被聘为中科院物理所杰出青年（B 类），教育部长江讲座教授（南京大学），南京大学思源教授，四川大学名誉教授，哈尔滨工业大学客座教授。