

Yanqi Molecular Science Forum 2019

雁栖分子科学论坛 2019

Program

会议日程

2019.7.5-2019.7.6

Beijing China

中国 北京

Organized by

School of Chemical Sciences, University of Chinese Academy of Sciences

Institute of Chemistry, Chinese Academy of Sciences

Co-organized by

Beijing National Laboratory for Molecular Sciences



雁栖分子科学论坛

“雁栖分子科学论坛”是由中国科学院大学（国科大）化学科学学院与中国科学院化学研究所（化学所）基于国科大暑期学校，共同发起与主办的国际学术论坛，是一个以国科大校园名称命名的高端学术交流平台。论坛旨在活跃化学科学学院和化学所的学术氛围，促进科教融合，培育研究生的创新意识，提升研究生的国际视野，培养一流创新型化学研究人才。“雁栖分子科学论坛”还旨在加强和促进国科大化学科学学院和化学所与国内外分子科学研究机构的学术交流和科技合作，繁荣分子科学的创新研究。自2018年起，“雁栖分子科学论坛”每年暑期在国科大雁栖湖校区国际会议中心举行。

国科大化学科学学院前身为中国科学院研究生院化学系，始建于1978年，是国科大主要基础学院之一。2014年，化学科学学院由化学所牵头承办，中科院与化学学科相关的京内外二十多个研究所以及校本部共同参与建设。2017年国科大化学学科入选教育部一流学科建设名单。





Yanqi Molecular Science Forum

Yanqi Molecular Science Forum is an international conference named after the Yanqi Lake campus of the University of Chinese Academy of Sciences (UCAS), and held annually at the International Conference Center of the Yanqi lake campus during the Summer semester since 2018. The Forum is organized jointly by the School of Chemical Sciences UCAS and Institute of Chemistry Chinese Academy of Sciences (ICCAS). The forum provides a platform for synergistic incorporation between ICCAS and the School of Chemical Sciences, as well as collaborations between these two institutions and international institutions/universities in chemical research. The forum also aims at helping graduate students to become first class researchers in Chemistry by boosting their enthusiasm in original research, and broadening their international horizon.

The School of Chemical Sciences of UCAS is previously known as the Department of Chemistry of Graduate University of Chinese Academy of Sciences (GUCAS) which was found in 1978, and is one of the major colleges in UCAS. Since 2014, the ICCAS is in charge of the teaching of the school of Chemical Sciences of UCAS, while more than 20 institutes related to chemistry of CAS participated. In 2017, the chemical sciences at UCAS is listed as first class by the Ministry of Education of China.



论坛组织

■ 论坛主席

张德清 范青华 周克斌 何圣贵

■ 组织委员会（以姓氏笔画为序）

主 任：范青华

副主任：周克斌

组委会成员：

王 树 李永舫 李向军 杨国强 杨镜奎 汪志祥 宋卫国

宋 锐 陈 义 何圣贵 范青华 孟丽萍 郑企雨 韩布兴

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中国科学院化学研究所

■ 协办单位

北京分子科学国家研究中心

Forum Organization

■ Forum Chairman

Deqing Zhang Qing-Hua Fan Kebin Zhou Shenggui He

■ Organizing Committees

Director: Qing-Hua Fan

Deputy Director: Kebin Zhou

Committee Members:

Shu Wang	Yongfang Li	Xiangjun Li	Guoqiang Yang
Jingkui Yang	Zhixiang Wang	Weiguo Song	Rui Song
Yi Chen	Shenggui He	Qing-Hua Fan	Liping Meng
Qiyu Zheng	Buxing Han		

■ Forum Working Group:

Cheng Peng (pengcheng@iccas.ac.cn)	Hua Tian (tianhua@iccas.ac.cn)
Xiaohang Zhang (zhangxh@ucas.ac.cn)	Bingjie Xu (xubingjie@ucas.ac.cn)

■ Organizers

School of Chemical Sciences, University of Chinese Academy of Sciences

Institute of Chemistry, Chinese Academy of Sciences

■ Co-organizer

Beijing National Laboratory for Molecular Sciences

PROGRAM

FRIDAY JULY 5

VENUE: Auditorium, UCAS International Conference Center

Session 1	
08:30-08:45	Chair: Qing-Hua Fan
08:30-08:45	Opening Remarks Deqing Zhang Institute of Chemistry, CAS
08:45-12:00	Chair: Shu Wang
08:45-09:45	Fluorescent Nucleosides, Nucleotides and Oligonucleotides Yitzhak Tor University of California, San Diego
09:45-10:45	Influencing Site Selectivity in the Cyclopalladation of 1-Naphthalenes and Related Substrates Gregory A. Solan University of Leicester
10:45-11:00	Coffee Break and Group Photo
11:00-12:00	Mass Spectrometry-Based Metabolomics and Imaging Analysis in Research of Environmental Toxicology Zongwei Cai Hong Kong Baptist University
12:00-13:30	Lunch
Session 2	
13:30-15:30	Chair: Shenggui He
13:30-14:30	Impacts of Molecular Optical Properties on External Quantum Efficiencies of Organic Light Emitting Devices Chung-Chih Wu Taiwan University
14:30-15:30	Conjugated Polymer-Based Assembly Materials for Biosensors and Beyond Shu Wang Institute of Chemistry, CAS
15:30-15:45	Coffee Break
15:45-17:45	Chair: Qiqiang Wang
15:45-16:45	Unnatural Synthetic Biology Jiangyun Wang Institute of Biophysics, CAS
16:45-17:45	Development and Application of Ring Formation Reactions Zhi-Xiang Yu Peking University
18:00-19:00	Dinner

PROGRAM

SATURDAY JULY 6

VENUE: Auditorium, UCAS International Conference Center

Session 1	
08:30-11:45	Chair: Deqing Zhang
08:30-09:30	Aggregation-Induced Emission: Embrace to the Poetry and the Lofty Benzhong Tang The Hong Kong University of Science and Technology
09:30-10:30	From Curved Polycyclic Aromatics To Electronic Materials Qian Miao The Chinese University of Hong Kong
10:45-11:00	Coffee Break
10:45-11:45	Artificial Photosynthesis for Chemical Transformation Li-Zhu Wu Technical Institute of Physics and Chemistry, CAS
12:00-13:30	Lunch
Session 2	
13:30-15:30	Chair: Qing-Hua Fan
13:30-14:30	Recent Research Progress of Photovoltaic Materials for Polymer Solar Cells Yongfang Li Institute of Chemistry, CAS
14:30-15:30	DNA Supramolecular Hydrogels Dongsheng Liu Tsinghua University
15:30-15:45	Coffee Break
15:45-17:45	Chair: Dexian Wang
15:45-16:45	Total Synthesis of Indole Alkaloids Enabled by Skeletal Reorganization Jieping Zhu École Polytechnique Fédérale de Lausanne (EPFL)
16:45-17:45	Bio-inspired Small Molecular Catalysis: Mechanism Oriented Catalyst Evolution Sanzhong Luo Tsinghua University
17:45-18:00	Closing Remarks
18:00-19:00	Dinner



ABSTRACTS



Yitzhak Tor

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➤ Educational Background

1982 B.Sc., Chemistry, Tel-Aviv University, Tel-Aviv, Israel
1990 Ph.D., Chemistry, The Weizmann Institute of Science, Rehovot, Israel
1993 Postdoctoral Fellow, California Institute of Technology, Pasadena, CA

➤ Professional Career

1993–1994 The University of Chicago: Assistant Professor of Chemistry.
1994–1999 The University of California, San Diego: Assistant Professor of Chemistry.
1999–2003 The University of California, San Diego: Associate Professor of Chemistry.
2003– The University of California, San Diego: Professor of Chemistry.

➤ Research Interests

Chemical biology of nucleic acid including antiviral and antibacterial agents; modified nucleosides and nucleotides; new emissive nucleosides and oligonucleotides; novel cellular delivery agents.

➤ Awards

1989 John F. Kennedy Prize for Distinguished Graduate Studies, Israel
1990/91 Weizmann and Weizmann–Bantrell Fellow, USA
1991 Gerhardt Schmidt Prize, Israel
1996 Hellman Faculty Fellow
2000 Project Kaleidoscope Faculty for the 21st Century
2006 Teddy G. Traylor Scholar in Organic Chemistry
2009 Lifetime Honorary Membership, Israel Chemical Society
2013 The George W. and Carol A. Lattimer Professorship

➤ Professional Service

2006–18 Founding Editor and Editor-in-Chief *Perspectives in Medicinal Chemistry*
2010 Member, NIH's College of Reviewers
2012 Co-Founder and organizer FB³ (Fluorescent Biomolecules and their Building Blocks)
2014– Permanent Steering committee MAF (Methods & Applications of Fluorescence)
2016 Member, Editorial Board, *The Journal of Antibiotics*
2016– Member, International Panel, *Volkswagen Foundation (VolkswagenStiftung)*
2018 Conference Chair, International Round Table on Nucleosides, Nucleotides and Nucleic Acids
2018– Section Editor (Structure determination/Chemical Synthesis), *Journal of Antibiotics*
2019 Conference Chair, Methods & Applications of Fluorescence (MAF 2019)

Fluorescent Nucleosides, Nucleotides and Oligonucleotides

Y. Tor

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Nucleic acids experience a variety of perturbations, which include strand cleavage and ligation, local conformational changes, base damage, modification and flipping, as well as structural and environmental perturbations that are induced upon protein and low MW ligand binding. Additionally, nucleosides and nucleotides are involved in numerous biochemical transformations and regulatory processes. Isomorphous responsive fluorescent nucleoside analogs, which can serve as faithful surrogates, are powerful probes for investigating nucleic acids structure, dynamics, recognition and damage as well as metabolic processes. Such modified nucleosides can also serve as mechanistic probes, shedding light on biological pathways and providing guiding design principles for potential therapeutics. The lecture will present the design and synthesis, as well as the structural and photophysical properties of new fluorescent isomorphous nucleoside analogs (Fig. 1) as well as their utilization for the fabrication of "real-time" fluorescence-based discovery and biophysical assays [1–12].

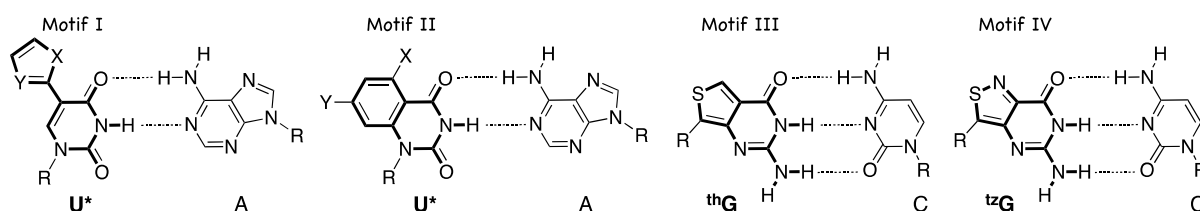


Fig. 1. Four motifs for emissive pyrimidine and purine analogs

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- [10] Y. Li, A. Fin, L. McCoy, Y. Tor, *Angew. Chem. Int. Ed.* **2017**, *56*, 1303.
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➤ Educational Background

- 1984-1988 **University of Sussex, UK.**
B.Sc. Hons. in Chemistry with European Studies (1st class honours).
- 1989-1992 **University of Cambridge, King's College, UK.**
Ph.D. 'The Elaboration of Bridging Ligands at Transition Metal Centres' (Supervisor: Dr. M. J. Mays).

➤ Professional Career

- 1988-1989 Research Chemist with Lilly Research Centre Limited, UK.
- 1993-1994 Postdoctoral Fellowship/Premier Assistant at the Université de Lausanne, Switzerland.
(with Prof C. Floriani).
- 1994-1996 Research Fellow at the University of Edinburgh (with Prof R. E. P. Winpenny).
- 1996-1997 Lecturer in Inorganic Chemistry at the University of Edinburgh.
- 1997-1998 Post-Doctoral Research Assistant; an Imperial College & BP Chemicals collaborative
research programme (with Prof V. C. Gibson).
- 1999-2007 Lecturer in Inorganic Chemistry at the University of Leicester.
- 2008- Associate Professor in Inorganic Chemistry at the University of Leicester.
- 2016-2018 Visiting Professor at the Institute of Chemistry, Chinese Academy of Sciences.

➤ Research Interests

Small molecule and polymerization catalysis. New metal catalysts for the synthesis of polyolefins and biodegradable polyesters. C-H activation and functionalization. New inorganic materials and magnetic properties. Organometallic and Coordination Chemistry. Sustainable catalysis. Catalytic mechanisms.

➤ Awards

- 2016 Fellow of the Higher Education Academy, UK
- 2001 ExxonMobil Chemical European Science and Engineering Award, Europe.

➤ Output

164 publications including research articles, book chapters, reviews and world patents. Citation index: 6014 (Scopus: June 2019). H-index 30 (Scopus: June 2019).

Influencing Site Selectivity in the Cyclopalladation of 1-Naphthalenes and Related Substrates

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Over the past decade a number of highly efficient synthetic strategies have been developed that involve the use of transition metal catalysts to directly cleave non-acidic C-H bonds, a process known as C-H activation.¹ Indeed, these reactions are revolutionizing organic synthesis because they can introduce a more atom economical first step in C-C and C-heteroatom bond forming processes, resulting in a more direct approach to the target transformation. However, despite the recent significant developments in the field of C-H functionalization, the control of site-selectivity remains a major challenge. Most commonly, a chelating directing group is employed to affect activation of a proximal C-H bond, typically at the *ortho*-site of an aromatic ring. Other factors have also been identified for the control of site-selectivity, including the innate reactivity of the substrate, the catalyst or metal-ligand combination and the solvent.

Herein we report a combined synthetic and computational study to ascertain the factors that influence the site-selectivity for C-H activation in a 1-naphthalene. In particular, we are interested in how cyclopalladation can be controlled to allow selectivity towards either *peri*- or *ortho*-activation of a pyridyl-imine substituted derivative.² While solvent plays a role, the nature of the intramolecular base and the chelation properties of the bidentate directing group are pivotal to the selectivity. Mechanisms based on a concerted metalation deprotonation (CMD)^{3a} or ambiphilic metal-ligand activation (AMLA)^{3b} are proposed and supported by DFT calculations.

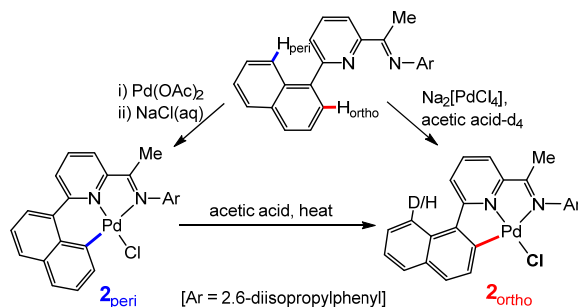


Fig. 1 Site selectivity in the cyclopalladation of 1-naphthalenes

References

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- [3] (a) M. Lafrance, K. Fagnou, *J. Am. Chem. Soc.*, **2006**, 128, 16496–16497; (b) D. L. Davies, S.M.A. Donald, S.A. Macgregor, *J. Am. Chem. Soc.*, **2005**, 127, 13754–13755.

Zongwei Cai

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➤ Educational Background

1978-1982 B.Sc., Xiamen University, China
1986-1990 PhD, University of Marburg, Germany

➤ Professional Career

2001-2005 Hong Kong Baptist University, Associate Professor
2005-2010 Hong Kong Baptist University, Professor
2010- Hong Kong Baptist University, Chair Professor

➤ Research Interests

The major research interest of Prof. Cai is method development and applications of chromatography coupled with mass spectrometry for trace analysis in complex systems such as environment, food and biological matrices, with focus on metabolomics and proteomics research on human health and diseases associated with environmental pollution.

➤ Awards

2018 Outstanding Contribution Award for the Elimination of Persistent Organic Pollutants
 (Chinese Society for Environmental Sciences)
2016 The 1st-grade Award from CAIA (China Association for Instrumental Analysis)
2011 The second prize in National Nature Science Award in 2011 (rank 5)

Mass Spectrometry-Based Metabolomics and Imaging Analysis in Research of Environmental Toxicology

Chao Zhao and Zongwei Cai*

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The effects of bisphenol S (BPS), an alternative to BPA, on breast tumor proliferation and deterioration were investigated. Potential molecular mechanisms via molecular biology and mass spectrometry-based lipidomics, proteomics and matrix-assisted laser desorption/ionization-MS imaging (MALDI-MSI) in human breast cancer xenograft model were studied. Oral exposure to mouse models with breast tumor xenograft at low (BPS-10: 10 µg/kg body weight/day) and high (BPS-100: 100 µg) levels were found to significantly promote proliferation of breast tumor. Our results demonstrated that BPS exposure remarkable perturbed abundances of 91 potential markers that mainly involved in five metabolic pathways. We elucidated the lipids spatial heterogeneity by using morphological analysis, probabilistic latent semantic analysis and co-registered multimodal three-dimensional (3D)-MSI. The obtained results suggested that BPS significantly induced tumor proliferation and heterogeneous by the variation of spatial distribution of proteins that were related to chromosomal stability and cell proliferation, lipids signaling, reprogramming of DNA methylation and hypoxic tumor microenvironment in central necrotic domains. BPS exposure caused the tumor deterioration by the variation of spatial distribution of proteins that were associated with the stability of nucleic acid structure, as well as structural lipids in peripheral neoplastic domains of breast tumor. Similar to BPA, BPS has growth-promoting effects on breast tumor in the mice model, which might increase the susceptibility of breast cancer. Furthermore, our results demonstrated the great potential of MALDI-MSI for morphology-driven toxicological evaluation induced by environmental pollutants.

References

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- [3] C. Zhao, Z. Tang, J. C. Yan, J. Fang, H. L. Wang, Z. W. Cai, *Sci. Total Environ.* **2017**, 592, 357-365.
- [4] Chao Zhao, Peisi Xie, Ting Yong, Hailin Wang, Arthur Chi Kong Chung, Zongwei Cai. *Anal Chem.* **2018** Feb 16. doi: 10.1021/acs.analchem.7b04540.

Chung-Chih Wu

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➤ Educational Background

1990	B.Sc., Taiwan University
1994	M.S., Princeton University
1997	Ph.D., Princeton University

➤ Professional Career

2019-	Department Chairman, Taiwan University, EE Dept.
2018-	Micron Technology Chair Professor, Taiwan University
2010-	Distinguished Professor, Taiwan University
2007-2010	Department Associate Chair, Taiwan University, EE Dept.
2006-	Professor, Taiwan University
2002-2006	Associate Professor, Taiwan University
1998-2002	Assistant Professor, Taiwan University
1997-1998	Research Scientist, ITRI

➤ Research Interests

Organic semiconductors for optoelectronics; oxide semiconductors/conductors and TFTs; displays; optics; transparent and flexible electronics; nano science and technologies;

➤ Awards

2001	NTU Outstanding Teaching Award
2003	Dr. Wu Da-You Research Award, National Science Council
2003	Outstanding Paper Award, Far Eastern Y.Z. Hsu Science and Technology Memorial Foundation
2004	Academia Sinica Young Scholar Award
2004	Outstanding Innovation Award, Industrial Technology Research Institute
2006	Distinguished Research Award, Ministry of Science and Technology (2006, 2009, 2012, 3 times)
2007	Distinguished Research Achievement Award, Taiwan University
2008	21 st Khwarizmi International Award (KIA)
2010	Distinguished Professor, Taiwan University
2011	Distinguished Electrical Engineering Professor, Chinese Institute of Electrical Engineering
2011	2011 Thomson Reuters Research Front Awards
2016	Fellow, Society for Information Display
2018	Micron Technologies Chair Professor, Taiwan University

Impacts of Molecular Optical Properties on External Quantum Efficiencies of Organic Light Emitting Devices

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In many OLED applications, power consumption and efficiency are a critical issue and thus achieving highest possible external quantum efficiency (EQE) of OLEDs is essential. To achieve ultimately high external quantum efficiencies of OLEDs, OLED materials and device architectures that can achieve high optical out-coupling efficiencies, together with other visual performance requirement, are equally important to those for internal quantum efficiencies. Although current OLEDs can offer nearly ~100% internal quantum efficiencies (IQEs), light extraction and out-coupling of internal emission remains a critical issue for achieving high and ultimate external quantum efficiencies (EQEs) and low power consumption for displays and lighting. In this presentation, we will discuss impacts of molecular optical properties on optical out-coupling efficiencies and external quantum efficiencies of OLEDs in the simple device configurations. These may include: (1) manipulation of emitting dipole orientations of OLED emitters, (2) low-refractive-index OLED active materials, (3) optically anisotropic OLED active materials, and (4) their combinations, for achieving optical out-coupling efficiencies and external quantum efficiencies of OLEDs in the simple device configurations.

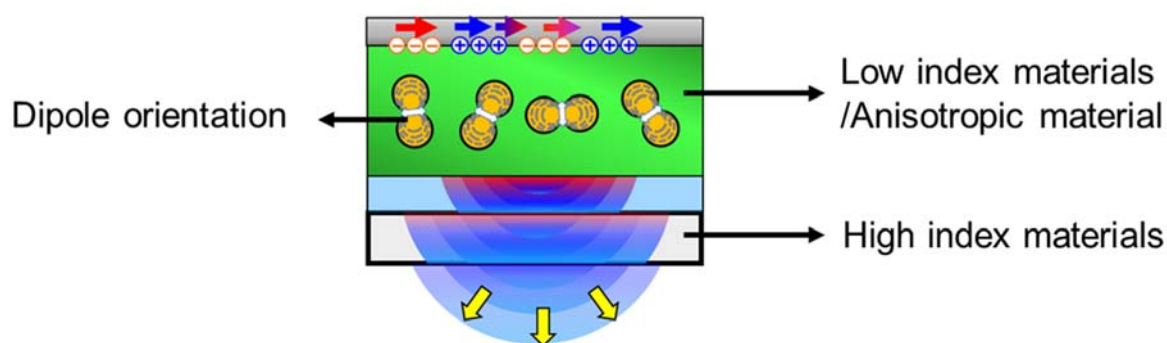


Fig. 1 Optical properties of OLED materials that will impact OLED optical efficiencies.

References

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- [5] W. Zeng, S. Gong, C.-C. Wu, C. Yang, et al., *Adv. Mater.* **2018**, 30, 1704961.

Shu Wang

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➤ Educational Background

1990-1994	B.Sc., Hebei University
1994-1999	Ph.D., Peking University

➤ Professional Career

1999.07-2001.07	Institute of Chemistry, Chinese Academy of Sciences	Postdoc
2001.10-2004.09	University of California at Santa Barbara	Postdoc
2004.10-	Institute of Chemistry, Chinese Academy of Sciences	Professor

➤ Research Interests

Design, synthesis and properties of light-harvesting conjugated polymers; Self-assembly biohybrid materials; Biosensors, cell imaging and disease therapeutic; Organic bioelectronics; Chemical biology

➤ Awards

2018-	Deputy Editor of ACS Applied Bio Materials
2006	Chinese Chemical Society Prize for Young Chemists
2007	National Natural Science Funds for Distinguished Young Scholars
2011	Chinese Academy of Sciences Award for Young Scientists
2011	Chinese Chemical Society–Royal Society of Chemistry Prize for Young Chemists
2011	The 12th National Award for Youth in Science and Technology of China
2013	Leading Talents of Technological Innovation of the Ministry of Science and Technology
2016	National “Ten Thousand Talent Program” Leading Talent
2013	Tarrant Visiting Professorship of Organic Chemistry of University of Florida
2014	The 2nd Ewha Distinguished Lectureship in Chemistry and Nano Science (Ewha Womans University, Korea)
2017-	Fellow of the Royal Society of Chemistry

Conjugated Polymer-Based Assembly Materials for Biosensors and Beyond

Shu Wang

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Water-soluble conjugated polymers (CPs) provide a unique platform for chemical and biological sensors in view of their optical signal amplification effect. Our recent studies showed that CPs/DNA complexes combining with fluorescence resonance energy transfer (FRET) processes could be used for detecting disease-related gene modifications, such as single nucleotide polymorphisms (SNPs), mutations and DNA methylation. In recent years, conjugated polymers (CPs) integrating recognition, imaging and therapeutic functions have attracted more and more attention. A novel photodynamic therapy (PDT) system was developed in which the photosensitizer is activated by chemical molecules instead of outer light source. In this system, luminol, hydrogen peroxide and horseradish peroxidase (HRP) were used as bioluminescent molecules and a cationic oligo (p-phenylene vinylene) (OPV) was used as the photosensitizer. The excited OPV by BRET from luminol sensitizes oxygen molecule in the surrounding to produce ROS that kill the adjacent cancer cells and pathogenic microbes. The BRET system can work in vivo even in the deeper tissue, which comes over the drawback of the deep tissue penetration for PDT with light irradiation. We designed an oligo(p-phenylenevinylene) unit with thiol groups and a paclitaxel unit (OPV-S-PTX). The OPV-S-PTX is capable of diffusing into cells, where π - π interactions lead to aggregation. Crosslinking of the aggregates via oxidation of thiol groups preferentially occurs inside tumor cells because of their higher internal reactive oxygen species (ROS) concentration. Crosslinked aggregates effectively “chemically lock” the multichromophore particle inside the cells and this process decreases the diffusion of the molecules out of the cell. The formation of the chemically locked particles enhances drug efficacy and helps in reducing resistance. Recently, we have also described a supramolecular antibiotic switch to reversibly “turn-on” and “turn-off” its antibacterial activity, which provides a proof-of-concept to regulate antibacterial activity and avoid accumulation of active antibiotics in the environment. This supramolecular antibiotic switch could be a potential strategy to fight bacterial infections and drug-resistance.

References

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➤ Educational Background

1994-1998 B.Sc., University of Science and Technology of China

1998-2003 Ph.D., University of Illinois at Urbana Champaign, Urbana

➤ Professional Career

2003-2007 The Scripps Research Institute Post-doc

2007- Institute of Biophysics, Chinese Academy of Sciences Principal Investigator

2015- University of Chinese Academy of Sciences Professor

➤ Research Interests

Chemical Biology; Synthetic biology; Biological physical chemistry

➤ Awards

2018 Innovative Talent Promotion Plan - Young and Middle-aged Talents in Science and Technology Innovation (Ministry of Science and Technology)

2016 5th CCS-RSC Young Chemist Award (CCS-RSC)

2015 Ten Thousand People Plan - Young Talents (Organization Department of the CPC Central Committee)

2015 Third Prize of Beijing Science and Technology Award (Beijing Municipal People's Government)

2015 Hundreds of millions of talent projects "Young and middle-aged experts with outstanding contributions" (Ministry of Human Resources and Social Security)

2015 The Changjiang Scholar Program-Youth Project (the Ministry of Education)

2014 Young Investigator Award of the Asian Photochemistry Society (APA)

2013 Young Science & Technology Award of China (Organization Department of the CPC Central Committee, Ministry of Human Resources and Social Security, China Science and Technology Association)

2013 China National Funds for Distinguished Young Scientists (NSFC)

Unnatural Synthetic Biology

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One aim in our laboratory is to use small, soluble protein scaffold, and the genetic incorporation of unnatural amino acid to design easy-to-characterize, easy-to-produce, and easy-to-optimize metalloenzymes which catalyze these important reactions with equal or greater efficiency/selectivity than that of the natural systems. Through the genetic incorporation of the Tyr-His ligand and CuB site into myoglobin, we recapitulated important features of HCO into this small soluble protein, which exhibits selective O₂ reduction activity while generating less than 6% ROS, at more than 1000 turnovers. These results support that Tyr-His crosslink is indeed important for HCO function, and creates the exciting opportunity to rapidly evolve better HCO model proteins to achieve higher activity and selectivity, which may be suitable as alternatives to precious metal catalyst in fuel cells.

Another aspect of our ongoing research is the development of new methods for precise attachment of functional metal complexes on biomolecules, which is an important strategy for metalloprotein design. Bioorthogonal chemical reactions together with genetic code expansion technique have provided exciting new means for protein labeling in living cells. The main advantages of photoclick reaction are its fast rate (up to 50 M⁻¹S⁻¹), and that it has no need for toxic copper catalyst.

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➤ Educational Background

1987-1991	B.Sc., Wuhan University
1994-1997	M.Sc., Peking University
1997-2001	Ph.D., Hong Kong University of Science & Technology

➤ Professional Career

2001.08-2004.05	UCLA, Postdoctoral Associate
2004.06-present	Peking University, Associate, full professor

➤ Research Interests

Computational and Synthetic Organic Chemistry: Joining Forces of Computation and Organic Synthesis to
1) Study Reaction Mechanisms; 2) Discover, Design and Develop New Reactions and Catalysts; 3)
Synthesize Natural and Non-Natural Products.

➤ Awards

2018	Wuxi Pharma Life Science Research Scholar Award
2018	Bayer Investigator Award at PKU
2016	Fellow of the Royal Society of Chemistry
2015	Chang-Jiang Professorship, Ministry of Education, China
2014	Nankai University Lectureship on Organic Chemistry
2012	Advisor of the Best 100 Ph.D Theses in China, Ministry of Education, China
2012	The Asian Core Program Lectureship Award (Singapore), the Asian Cutting-Edge Organic Chemistry programs
2011	"Chinese Chemical Society-Sci Finder Award for Creative Work in Synthetic Organic Chemistry"
2011	"Chinese Chemical Society-Physical Organic Chemistry Award"
2011	"Chinese Chemical Society-BASF Award"
2010	"Distinguished Lectureship Award", the Asian Symposium of Annual Meeting of Chemical Society of Japan
2008	The Asian Core Program Lectureship Award (Japan), the Asian Cutting-Edge Organic Chemistry programs
2008	The National Science Fund for Distinguished Young Scholars of China
2008	The Young Chemist Award, the Chinese Chemical Society & the Royal Society of Chemistry
2008	Thieme Synlett/Synthesis Journal Award

Development and Application of Ring Formation Reactions

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One of the research interests in Yu group at Peking University is developing ring formation reactions and applying these reactions to the synthesis of natural products and pharmaceuticals. Some of these ring formation reactions catalyzed by Rh complexes discovered in the Yu group have been shown in the scheme below. In this talk, recent progresses will be presented.

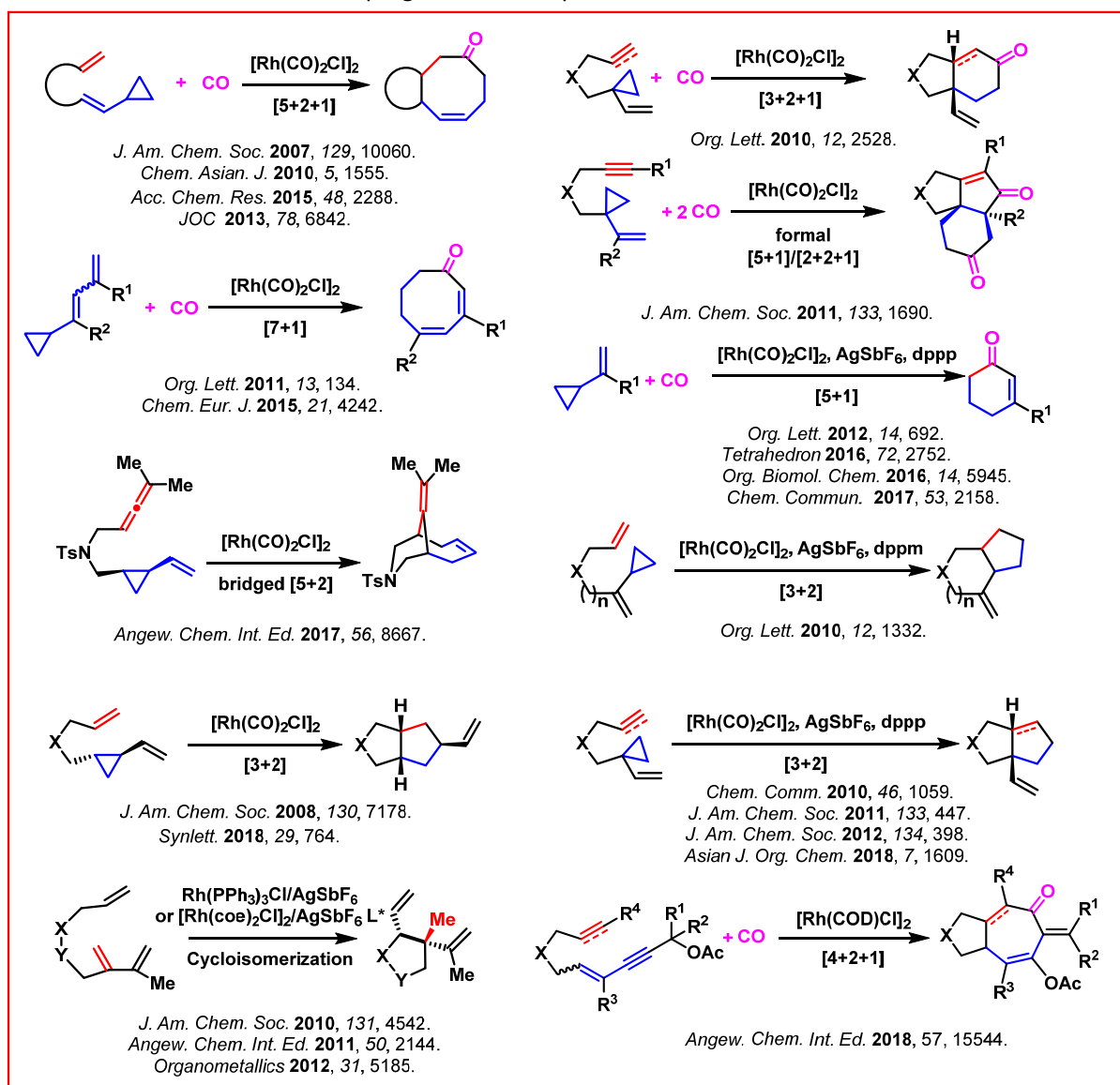


Fig. 1 Ring Formation Reactions Discovered in the Zhi-Xiang Yu Group

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➤ Educational Background

1978-1982	BS , South China University of Technology
1983-1985	MS , Kyoto University
1985-1988	Ph.D , Kyoto University

➤ Professional Career

2000-2005	The Hong Kong University of Science & Technology,	Associate Professor
2005-2008	The Hong Kong University of Science & Technology,	Professor
2008-	The Hong Kong University of Science & Technology,	Chair Professor
2017-	SCUT-HKUST Joint Research Institute,	Dean

➤ Research Interests

Exploration of polymer synthesis methodology, development of advanced functional materials and study of aggregation-induced emission

➤ Awards

2018	State Natural Science Award, 1st Class
2017	HLHL Foundation for Scientific and Technological Progress Award (The Ho Leung Ho Lee Foundation)
2017	Excellent Member of Editorial Board, <i>Science China: Chemistry</i>
2016	Outstanding Contribution Award, <i>Science China Chemistry</i>
2015	Honorary Citizen of the City of Guangzhou
2015	Best Paper Award, <i>Science China: Chemistry</i>

Aggregation-Induced Emission: Embrace to the Poetry and the Lofty

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Scientists are poets. A scientific concept is a poem describing some natural phenomena, which plays a critical role in the development of a new subject. Before the birth of AIE, the concept of aggregation-caused quenching (ACQ) effect is considered as a general belief and a well-accepted concept for common organic luminophores. The ACQ concept has reformed peoples' idea that the aggregation is harmful for solid-state light emission. The long standing and established concept restricts people's way of thinking and a novel concept is highly demanded to reform people's mind and guide the research. Our group started from occasional interesting findings and has established the concept of Aggregation-induced emission (AIE) in 2001, which provides a new platform for luminophore research.^[1-2] During 17 years of AIE research, the mechanism has evolved from restriction of intramolecular rotation (RIR) to restriction of intramolecular motion (RIM) and to recently the concept of through-space conjugation together with the through-bond conjugations, the emission types has ranged from solid-state fluorescence to room-temperature phosphorescence and further to aggregation-induced delayed fluorescence (AIDF), the luminophores has changed from traditional luminophores to nonconventional luminogens. AIE has established a new platform in the area for novel luminogen exploration and for multidiscipline researchers to work on. Diverse AIE luminogens with tunable color and high quantum yields have been explored, which finds diverse applications from optics and electronics to energy, environment and bioscience. Most importantly, the concept of AIE has gradually changed people's thinking way about the aggregation of luminogen and put forth a revolution of luminogen research both conceptually and technically. In this talk, I will share with you our journey of AIE research, discusses our current understanding of the AIE mechanism, debates current challenges, looks for the potential breakthroughs in this exciting research area,^[3] and embrace to the poetry and the lofty of AIE.

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➤ Educational Background

2000 B. Sc., University of Science and Technology of China

2005 Ph. D, Columbia University

➤ Professional Career

2005-2006 University of California, Los Angeles Postdoctoral Scholar

2006-2012 The Chinese University of Hong Kong Assistant Professor

2012-2016 The Chinese University of Hong Kong Associate Professor

2016- The Chinese University of Hong Kong Professor

➤ Research Interests

Design and synthesis of novel polycyclic aromatic molecules with interesting structures and useful applications, and development of high-performance organic semiconductor materials and devices using tools from organic synthesis, supramolecular chemistry and surface chemistry.

➤ Awards

2018 Croucher Senior Research Fellowship, Croucher Foundation, Hong Kong

2017 Research Excellence Award 2016-17, the Chinese University of Hong Kong

2012 Young Researcher Award 2011, the Chinese University of Hong Kong

2005 The Hammet Award, the Department of Chemistry, Columbia University

From Curved Polycyclic Aromatics To Electronic Materials

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Curved polycyclic arenes are not only unique objects of structural organic chemistry in relation to the nature of aromaticity, but also play an important role in science of carbon nanomaterials and organic functional materials. This lecture will present the synthesis and applications of three types of curved polycyclic aromatics that were designed by my research group. The first type is negatively curved polycyclic arenes containing seven- or eight-membered rings.^[1] They are not only segments but also synthetic precursors for theoretical carbon allotropes of negative curvature, which are known as Mackay crystals or carbon Schwarzites. The second type is carbon nanobelts that represent sidewall segments of armchair and chiral single-wall carbon nanotubes.^[2] The recently achieved synthesis of these carbon nanobelts is a key step towards ultimate bottom-up synthesis of uniform carbon nanotubes of single chirality and predefined diameter. The third type is organic semiconductors based on twisted hexabenzoperylenes (HBPs). Functionalized HBPs present an unusual type of π -stacking that allows a variety of functional groups to be grafted onto organic semiconductors without sacrificing π - π interactions in the solid state. This unprecedented supramolecular platform, in a device integrating an organic field effect transistor channel and a microfluidic channel, has enabled electronic sensors for highly sensitive and selective detection of chemical and biological species.^[3]

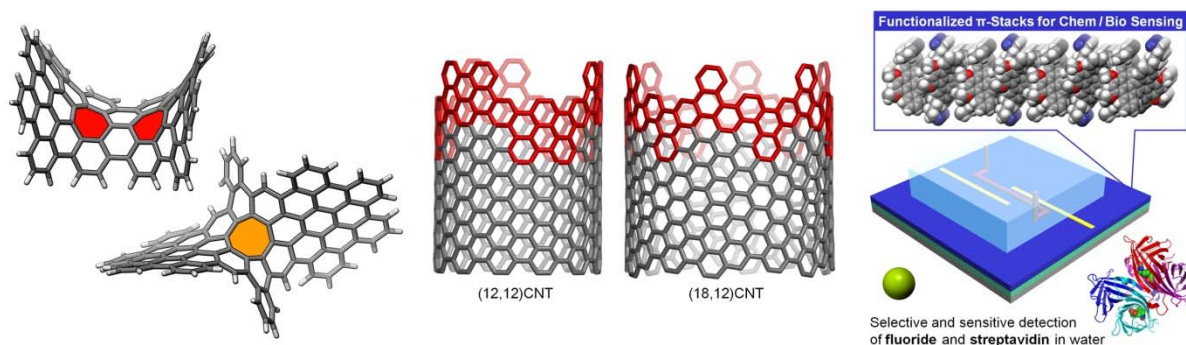


Fig. 1 Structures of three types of curved polycyclic aromatics

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➤ **Scientific Vita**

- 1999- Professor of Chemistry, Technical Institute of Physics and Chemistry, CAS
- 1997-1998 Post-doc, The University of Hong Kong (Supervisor: Prof. Chi-Ming Che)
- 1996-1999 Associate professor, Institute of Photographic Chemistry, CAS
- 1995-1996 Assistant professor, Institute of Photographic Chemistry, CAS
- 1990-1995 Ph.D, Institute of Photographic Chemistry, CAS (Supervisor: Prof. Chen-Ho Tung)
- 1986-1990 B.Sc., Department of Chemistry, Lanzhou University

➤ **Research Interests**

Her research interests are focused on photochemical conversion, including artificial photosynthesis, visible light catalysis for organic transformation, and photoinduced electron transfer, energy transfer and chemical reactions in supramolecular systems.

➤ **Awards**

- 2001 The National Nature Science Fund for Distinguished Young Scholar
- 2004 New Century Talents Project
- 2005 The 2nd prize of National Natural Science Award as second principal investigator
- 2006 "Hundred Talents Program" of the Chinese Academy of Sciences
- 2007 The 10th China Youth Science and Technology Award
- 2009 The 3rd Ten Outstanding Women of the Chinese Academy of Sciences
- 2010 The 7th Young Women Scientists Award of China
- 2013 The Prize of 10th Physical Organic Chemistry
- 2014 "Outstanding Graduate Teacher" award
- 2016 The 3rd Chinese Chemical Society-Evonik Chemical Innovation Award
- 2016 "National Million People Plan" Million Project Leader

Artificial Photosynthesis for Chemical Transformation

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Inspired by the ability of natural photosynthesis to convert solar energy into chemical energy, the scientific community long ago recognized the potential of light-driven reactions (photochemistry) as a powerful approach to chemical synthesis. From the high energy intermediate generated by photoinduced excitation of organic molecules, unique reaction manifolds can be accessed that are generally unavailable to conventional thermal pathways. Thus photochemical reactions considerably enrich the synthetic repertoire of modern organic chemists. Our group has long engaged in the photochemistry research related to the photoinduced energy transfer, electron transfer and chemical transformation. In this presentation, we will compile several stories to illustrate photochemical approaches that may be useful in the design of artificial photosynthetic systems for effective chemical transformation.

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➤ Educational Background

1978-1979	Undergraduate, East China University of Science and Technology
1979-1982	MS., East China University of Science and Technology
1983-1986	Ph.D., Fudan University

➤ Professional Career

1986-1988	Postdoctoral fellow, Institute of Chemistry, Chinese Academy of Sciences (ICCAS)
1988-	Staff of ICCAS, 1991.12-1993.11, Associate Professor; 1993.12-present, Professor

➤ Research Interests

Photovoltaic materials and devices for polymer solar cells, optoelectronic conjugated polymers, electrochemistry of conducting polymers.

➤ Awards

1995	Winning the <i>Second-Grade National Award of China on Natural Sciences</i> , for the contribution in "The studies on conducting polypyrrole"
1998	Named as " <i>Young and Middle-aged Specialist with Outstanding Contributions in Natural Science</i> " by Chinese government.
2005	Winning the <i>First-Grade Award of Beijing City on Science and Technology</i> , for the contribution in "The studies on the electrochemistry of conducting polymers and polymer light-emitting electrochemical cells".
2012	Winning "Macro2012 Lecture Award" by PMSE of ACS (American Chemical Society).
2018	Winning the <i>Second-Grade National Award of China on Natural Sciences</i> , for the contribution in "Photovoltaic materials of conjugated polymer donors with conjugated side chains and indene-fullerene bisadduct acceptors".
2018	Winning the <i>Second-Grade Award of Beijing City on Science and Technology</i> , for the contribution in "Controllable synthesis of colloid quantum dots and their application in high quality light-emitting diodes".

Recent research progress of photovoltaic materials for polymer solar cells

Yongfang Li

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Polymer solar cells (PSCs) have attracted great attention in the past decade, because of the advantages of simple device structure, light weight and capability to be fabricated into flexible and semitransparent devices. The key photovoltaic materials of PSCs are conjugated polymer donors and *n*-type organic semiconductor (*n*-OS) acceptors. Recently, the low bandgap *n*-OS acceptors (such as ITIC) have promoted the research progress of the PSCs significantly. Here I will report our recent research progress on the polymer donors to match with the narrow bandgap *n*-OS acceptor and the new *n*-OS acceptors. We developed a series of medium bandgap 2D-conjugated D-A copolymer donors based on bithienyl-benzodithiophene (BDTT) as donor unit and fluorobenzotriazole (FBTA) as acceptor unit. The D-A copolymer donors possess complementary absorption spectra and matching electronic energy levels with ITIC acceptor. By side chain engineering (alkyl-thienyl, alkylthio-thienyl, trialkylsilyl-thienyl¹ or alkyl-difluorothienyl² substitution) on the thiophene conjugated side chains of the polymers, the power conversion efficiency (PCE) of the PSCs with the polymers as donor and ITIC as acceptor reached 9.26%~11.63%². By side chain isomerization of ITIC, the PCE of the PSCs was further improved to 11.77%³~12.05%⁴. In addition, we designed and synthesized a low cost polymer donor PTQ10 which shows a high PCE of 12.7% when using a narrow bandgap *n*-OS IDIC as acceptor.⁵ Furthermore, we simplified the synthetic steps for the central core of IDIC and synthesized new and low cost acceptors MO-IDIC and MO-IDIC-2F which showed PCE of 13.46% when blending with PTQ10 as donor.⁶

References

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- [4] H. Bin, Y. K. Yang, Z. Peng, L. Ye, J. Yao, L. Zhong, C. Sun, L. Gao, H. Huang, X. Li, B. Qiu, L. Xue, Z.-G. Zhang, H. Ade, Y. F. Li, *Adv. Energy Mater.*, **2017**, *7*, 1702324.
- [5] C. Sun, F. Pan, H. Bin, J. Zhang, L. Xue, B. Qiu, Z. Wei, Z.-G. Zhang, Y. F. Li, *Nature Commun.*, **2018**, *9*, 743.
- [6] X. Li, F. Pan, C. Sun, M. Zhang, Z. Wang, J. Du, J. Wang, M. Xiao, L. Xue, Z.-G. Zhang, C. Zhang, F. Liu, Y. F. Li, *Nat. Commun.*, **2019**, *10*, 519.

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➤ Educational Background

1988-1993 B.Sc., University of Science and Technology of China
1999-2002 Ph.D., The Hong Kong Polytechnic University

➤ Professional Career

1993-1999 Institute of Chemistry, Chinese Academy of Sciences, Research Assistant/Associate
2003-2005 University of Cambridge, Postdoc Research Associate
2005-2009 National Centre for NanoScience & Technology, China Principle Investigator, Professor
2009- Tsinghua University, Professor

➤ Research Interests

We are interested in using biomolecules and their specific interaction in nanostructure fabrication and nanodevice design, which include:

1. DNA Nanotechnology: Nanostructures based on DNA self-assembly; Concept and running mechanism studies of DNA nanomachines; Nanochannel, Nanocontainer and smart surface based on DNA nanomachines;
2. Frame Guided Assembly: Methodology and its application in preparing shape and size controllable vesicles at nanometer scale;
3. Supramolecular Hydrogels based on DNA Self-assembly: fabrication, characterization and their application in 3D Bioprinting and tissue engineering.

➤ Awards

2009 The First CCS-RSC Young Scientist Award
2011 Fellow of Royal Society of Chemistry (FRSC)
2014 The 7th CCS-BASF Youth Innovation Prize
2016 Chang Jiang Scholars

DNA Supramolecular Hydrogels

Dongsheng LIU

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The reversible responsiveness of DNA secondary structures to environmental stimuli has enabled to facilitate responsive devices and materials based on pure DNA or hybrid systems. Based on sequence and structure design, we have prepared kinds of pure or hybrid DNA supramolecular hydrogels, which could be formed under physiological condition within a minute at room temperature and without using any organic solvents. By tailoring the length of “sticky ends” of DNA linker, mechanical property of the hydrogel could be varied from hundreds to thousands Pa (G' , storage modulus); we also found that the viability of cell in a 4 mm diameter hydrogel is nearly 100% after 24 hours incubation from top in plastic tubes. These hydrogels possess extraordinary healing and fast-responding thixotropic properties, which make them injectable and writable. Because the formations of such hydrogels are based on DNA assembly, by DNA sequence design, they could be easily conferred excellent responsiveness including pH, DNA restriction enzymes, temperature etc., and enable easy removal after cell culture. In addition, we will show their application in 3D cell printing.

References

- [1] Y. Shao, H. Jia, T. Cao and D. Liu* *Acc. Chem. Res.*, **2017**, *50*, 659–668.
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➤ Educational Background

- 1980-1984 B. Sc., Hangzhou Normal University
- 1984-1987 M. Sc., Lanzhou University (Advisor: Prof. Y.-L. Li)
- 1988-1991 Ph. D, Institut de Chimie des Substances Naturelles, CNRS, France (Advisors: Prof. H.-P. Husson, Prof. J.-C. Quirion)
- 1991-1992 Schering-Plough Post-doctoral fellow, Texas A & M University, USA (Advisor: Prof. D. H. R. Barton)

➤ Professional Career

- 1992-2000 Chargé de Recherche, CNRS, France
- 2000-2006 Director of Research, 2nd class, CNRS, France
- 2006-2010 Director of Research, 1st class, CNRS, France
- 2010- Professor, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

➤ Research Interests

Total synthesis of natural products, Multicomponent reaction, Metal-catalyzed Domino process, Catalytic enantioselective transformation.

➤ Awards

- 2017 KAIST-BK21 School of Molecular Science Lectureship award, South Korea
- 2016 Royal Society of Chemistry (RSC) Natural Product Chemistry Award, UK
- 2015 Nankai University Lectureship on Organic Chemistry, Nankai University, P. R. China
- 2010 French Chemical Society-Division of Organic Chemistry SCF-DCO award, France.
- 2009 Silver medal of CNRS, France
- 2008 Novartis Chemistry Lectureship, Switzerland
- 2004 Liebig Lectureship of German Chemical Society, Germany
- 2003 Prix "Emile Jungfleisch" of French Academy of Science, France
- 2003 Outstanding Young Oversea Scientist Award (NSFC), P. R. China
- 2002 AstraZeneca Awards in Organic Chemistry, UK.
- 2002 JSPS (Japan Society for Promotion of Science) Research Fellow, Japan.
- 1999 French Chemical Society-Division of Organic Chemistry, SFC-ACROS award, France
- 1996 Bronze Medal of CNRS, France.

Total Synthesis of Indole Alkaloids Enabled by Skeletal Reorganization

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Rearrangement is a broad class of organic transformations involving the migration of an atom or a group from one center (migration origin) to another (migration terminus) within the same molecule. Such bond reorganization process affords a structural isomer of the original substrate allowing, in many cases, the construction of molecular frameworks not easily accessible by other approaches. Incorporation of a rearrangement reaction in a domino sequence will without doubt further increase the structure complexity and diversity of the reaction product. In this talk, we will present our recent work on the total synthesis of polycyclic indole alkaloids featuring 1,2-alkyl migration as a strategic reaction.^[1,2]

References

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➤ Scientific Vita

1995-1999	B.A, Zhengzhou University
1999-2002	M.S., Nankai University (supervisor: Prof. Jin-Pei Cheng)
2002-2005	Ph.D., ICCAS (supervisor: Prof. Jin-Pei Cheng)
2005-2018	Assistant/Associate/full Professor, Institute of Chemistry, CASciences
2018-present	Professor, Tsinghua University

➤ Research Interests

Bio-inspired catalysis and synthesis, physical organic chemistry and supramolecular catalysis/synthesis

➤ Awards and Recognition

2018	Innovation Leading Scholar, National Ten-thousands Program
2017	POC Youth Award of Chinese Chemical Society
2016	Chiral Youth Award of Chinese Chemical Society (CCS)
2014	National May 4 th Youth Medal ("Wu Si" Medal)
2014	Innovation Award for Teaching, ICCAS
2013	Excellence in Research and Management, CAS Beijing Division
2012	National Program for Support of Top-notch Young Professionals
2012	Thieme Journal Award;
2011	elected President of Youth Innovation Promotion Association, CAS (2013, re-elected)
2011	Asia Core Program Lectureship
2010	National Science Fund for Distinguished Young Scholar
2009	Lu Jiaxi Young Scientist Award of the Chinese Academy of Science
2008	Young Chemist Award of the Chinese Chemical Society
2007	Rising Star of Science and Technology Research in Beijing

Bio-inspired Small Molecular Catalysis: Mechanism Oriented Catalyst

Evolution

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Enzymatic catalysis is an essential tool for new matters and functions in Nature, hence serves as inspiring resources for new reactions and catalysis in chemistry. To develop new catalysts/ligands with superior performance and broad applicability remains a central theme in asymmetric catalysis. Inspired by Nature, we have developed bio-inspired small molecular catalysts as both functional and mechanistic enzyme mimics,¹ showing unprecedented scopes in fundamental transformations of carbonyls and olefins.^{2,3} Systematic physical organic studies, combining both experimental and theoretical approaches including DFT calculations and machine learning, have been shown to aid in the understanding of catalytic mechanism and in the evolution of new catalyst. In this talk, I'll present our recent advances along this line.

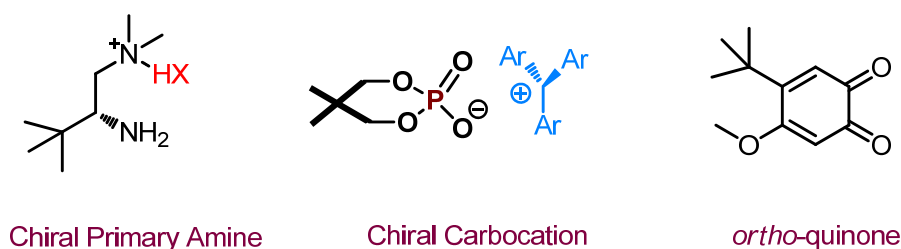


Fig. 1 Bio-inspired small molecular catalysts

References

- [1] (a) Zhang, L.; Luo, S. *Acc. Chem. Res.* **2015**, *48*, 986. (b) Zhang, L.; Luo, S. *Synlett* **2012**, 1575-1589. (c) Lv, J.; Luo, S. *Z. Chem. Commun.* **2013**, *49*, 847. (d) Qin, Y.; Zhu, L.; Luo, S. *Z. Chem. Rev.* **2017**, *117*, 9433. (e) Zhang, R. P.; Luo, S. *Z. Chin. Chem. Lett.* **2018**, *29*, 1193.

University of Chinese Academy of Sciences Yanqi Lake Campus Map



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