西湖大學
WESTLAKE UNIVERSITY

WORLD YOUNG
SCIENTIST SUMMIT
世界青年科学家峰会

2021WE论坛
前沿合成与功能分子分论坛

2021 WE Forum of Westlake University
Discovery, Design and Synthesis of Functional Molecules Symposium

会议手册
PROGRAM

主办单位
西湖大学 | 浙江省科学技术协会 | 温州市人民政府

Organizers
Westlake University | Zhejiang Association for Science and Technology
Wenzhou Municipal People's Government

2021年10月26-27日　中国 · 杭州
October 26th-27th, 2021　Hangzhou, China

Contents（目录）

About the 2021 WE Forum

The World Young Scientist Summit (WYSS) as an academic event held once a year for the world young talents is jointly sponsored by the China Association for Science and Technology (CAST) and the People's Government of Zhejiang Province. With its long-term vision for building a community of common destiny for all humanities, WYSS sets on the Converging the World's Talents Creating a Better Future theme; oriented for one global vision with international interests and a China voice, WYSS attracts talents from all corners of the world for their dreams in sciences. In acknowledging ‘the future of science and technology is dependent of our young’ being the global and century concerns, WYSS highlights its main discussion premise around world’s young scientists with integrated interest from industries, venture capitals, arts and other societal endeavors. It has led to another improvement in academic and cultural exchanges, enabled leadership from world’s top scientist, offered enhanced participations from young scientists and involved private entrepreneurs, to jointly address global challenges, establish a platform for talent exchange in a wider range of fields and provide a carrier of higher-level scientific and technological innovation.

The first WYSS was held with great success in Wenzhou, China, in October 2019.

Westlake University, established in 2018, is a new type of research university, a first in the history of modern China. It enjoys strong public support and aims to be a reformer in our higher education system. Westlake University is striving to cultivate top talent, to make breakthroughs in basic research and innovation in cutting-edge technologies, and to foster human development through science and technology. Founded by prominent scientists and scholars, Westlake University is committed to building a truly international, world leading, research-focused university.

The WE Forum is an international academic symposium held by Westlake University since 2018. WE is the abbreviation of “Westlake Education” and the short name for “Westlake Education Foundation”, which is the fund-raising body of Westlake University. It implies that Westlake University will focus on academic development to achieve its mission on higher education reforms and development. WE also means you and me, implying academics are closely linked with each other. WE forum emphasizes the importance of people in academic exchanges and advocates global scholars to be participants, sharers, and contributors of academic exchanges.

In August 2021, the Secretariat of World Young Scientist Summit (WYSS) and Westlake University signed an agreement to enhance collaboration, in which the WE Forum was officially listed in the programs of WYSS.

As one of the sub-forums in 2021 WE Forum, **the Discovery, Design and Synthesis of Functional Molecules Symposium** aims to provide an exchange platform for researchers to share knowledge and research findings, discuss existing challenges, and explore exciting new ideas and cutting-edge technologies. It will offer various talks from established chemists of academic leaders. The conference will focus on four fields: Synthetic Chemistry, Energy Chemistry, Chemical Biology, and Physical Chemistry.

The experts and graduate students who are engaged in related fields are warmly welcomed to participate in this symposium. Our symposium provides a venue for an extensive and in-depth discussion on the new achievements and progress in chemistry or related fields.

Time： October 26th - 27th, 2021
Venue： Hangzhou Narada Resort & Spa Liangzhu, Zhejiang, China
Sponsors: China Association for Science and Technology (CAST), The People’s Government of Zhejiang Province
Organizer: Westlake University, Zhejiang Association for Science and Technology, Wenzhou Municipal People's Government

关于本论坛

世界青年科学家峰会是中国科学技术协会与浙江省人民政府共同发起、联合主办的面向全球青年高层次人才的活动，每年举办一次。峰会以推动人类命运共同体建设为愿景目标，围绕“汇聚天下英才共创美好未来”主题，把握“全球视野、国际议题、中国声音”要求，根据“科技的未来在青年”这一全球性、时代性主题，开展国际科技人文交流，让顶尖科学家高端引领、让青年科学家深度参与、让民营企业家精准对接，共同应对全球性挑战，打造更宽领域人才交流平台、更高能级科技创新载体。

西湖大学是一所社会力量举办、国家重点支持的新型高等学校，于2018年2月14日正式获教育部批准设立，致力于集聚一流师资、打造一流学科、培育一流人才、产出一流成果，努力为国家科教兴国和创新驱动发展战略作出突出贡献，立志成为人类文明的重要创新引擎和孵化器。学校坚持“高起点、小而精、研究型”的办学定位，积极探索适合中国国情的新型研究型大学治理制度和鼓励原始创新的新型科技评价制度，聚焦基础前沿科学研究，注重学科交叉融合，取得了一系列具有影响力的科技创新成果。

WE 论坛（WE Forum）是西湖大学主办的大型国际性学术论坛，首届论坛于2018年10月举办。WE是Westlake Education的缩写，同时，也是中文“我们”的意思。WE论坛寓意西湖大学以学术研究为根本、促进教育事业的发展。同时，WE论坛强调人在学术交流中的重要性，倡导全球学人做学术交流的参与者、分享者和贡献者。

2021年8月，世界青年科学家峰会执委会与西湖大学签署合作协议，深化合作，在世界青年科学家峰会框架下共同举办好WE论坛。

2021 WE 论坛将主题确定为“加强合作，共谋未来”，旨在通过学术交流推动世界各国青年科学家的交流与合作。论坛设一个主论坛、四个分论坛，聚焦生命科学、智能科学、微纳加工、先进材料、环境资源、前沿合成与功能分子、量子物质和量子信息等学科前沿领域。

其中，**前沿合成与功能分子分论坛**作为 2021 WE 论坛的分论坛之一，主要聚焦于化学合成领域的前沿科学问题与挑战，从反应历程探索、新催化剂开发、新合成及检测方法建立，到功能分子合成、应用研究，系统性地分享最新的科研成果。本论坛旨在为从事化学研究的科研工作者提供交流平台，通过思想碰撞促进相互借鉴学习、建立共赢的合作关系。

组委会热诚欢迎从事相关领域研究的专家、研究生参加本次研讨会，就化学及相关领域的新成就和新进展进行广泛而深入地交流与探讨。

时　　间：2021 年 10 月 26 日-27 日
地　　点：浙江省杭州市良渚君澜酒店
指导单位：中国科学技术协会、浙江省人民政府
主办单位：西湖大学、浙江省科学技术协会、温州市人民政府

Agenda（日程）

Discovery, Design and Synthesis of Functional Molecules Symposium

- Junlan Ballroom, Hangzhou Narada Resort & Spa Liangzhu -
- 杭州良渚君澜酒店，君澜厅 –

October 26th, Tuesday, Day 1	
08:30-08:40	Welcome Remarks
Session I	Chair: Dr. Zhichang Liu (PI of School of Science, Westlake University)
08:40-10:20	**Construction of Zigzag Hydrocarbon Belts–An Organic Chemist's Perspective on Carbon Nanostructures** Speaker 1: Meixiang Wang (Tsinghua University)
	Understanding Carrier Transfer Across Interfaces in Metal Halide Perovskites Speaker 2: Juan-Pablo Correa-Baena（Georgia Institute of Technology, USA）*Online*
	Synthesis and Imbalanced C–H Activation Reactivity of a Terminal Co Oxo Complex Speaker 3: John Anderson（University of Chicago, USA）*Online*
10:20-10:50	Photo-Taking / Refreshment Break
Session II	Chair: Dr. Lihan Zhang (PI of School of Science, Westlake University)
10:50-12:20	**Combining Synthetic Chemistry and Biology for Streamlining Access to Complex Molecules** Speaker 4: Hans Renata（The Scripps Research Institute, USA）*Online*
	Lecture 5 (为合成科学插上化学与生物两只翅膀) Speaker 5: Xiaoguang Lei (Peking University)
	Chemical Proteomic Profiling of Functional Modifications by Reactive Metabolites Speaker 6: Chu Wang (Peking University)
12:20-13:50	Buffet & Lunch Break
Session III	Chair: Dr. Haihua Lu (PI of School of Science, Westlake University)
13:50-15:00	***Exo*-Selective Diels–Alder Reactions Enabled by a Bispyrrolidine Diboronate** Speaker 7: Zhen Yang (Peking University)
	Lecture 8 (含氟复杂分子的合成研究) Speaker 8: Pingping Tang (Nankai University)
15:00-18:00	Free Tour
18:00-20:00	Welcome Dinner

October 27th, Wednesday, Day 2

Session IV	Chair: Dr. Zhaobin Wang (PI of School of Science, Westlake University)
08:30-10:10	**Lecture 9 (有机功能染料与产品工程)** Speaker 9: Weihong Zhu (East China University of Science and Technology)
	Nickel-Mediated Radical Pathways and Applications in *C*-Glycosylation Speaker 10: Tianning Diao (New York University, USA) *Online*
	Lecture 11 (手性 Lewis 碱和过渡金属协同不对称催化) Speaker 11: Liuzhu Gong (University of Science and Technology of China)
10:10-10:30	Refreshment Break
Session V	Chair: Dr. Huaimin Wang (PI of School of Science, Westlake University)
10:30-12:00	**Discovery and Biosynthesis of Marine Actinobacteria-Derived Polycyclic Natural Products** Speaker 12: Changsheng Zhang (South China Sea Institute of Oceanology)
	Lecture 13 (时空分辨的生物正交反应及分子探针) Speaker 13: Yan Zhang (Nanjing University)
	Lecture 14 (无机磷材料的化学生物学研究) Speaker 14: Jing Zhao (Nanjing University) *Online*
12:00-13:30	Buffet & Lunch Break
Session VI	Chair: Dr. Wenjie Dou (PI of School of Science, Westlake University)
13:30-15:10	**Molecular Materials Property Prediction: Mechanism and Computational Methods** Speaker 15: Zhigang Shuai (Tsinghua University)
	Visualizing a Single Molecule at the Single-Bond Limit Speaker 16: Yi Luo (University of Science and Technology of China)
	Lecture 17 (多孔芳香骨架材料-PAFs) Speaker 17: Guangshan Zhu (Northeast Normal University)
15:10-15:30	Refreshment Break
Session VII	Chair: Dr. Biaobiao Zhang (PI of School of Science, Westlake University)
15:30-17:10	***In Situ* Neutron Measurements in Materials Chemistry** Speaker 18: Howard Wang (University of Maryland, College Park, USA)
	Dynamics and Mechanism of Water Oxidation Catalysts Speaker 19: Mårten S. G. Ahlquist（Royal Institute of Technology, Sweden）*Online*
	The Coalescence Behavior of Two-Dimensional Materials Revealed by Multiscale *In Situ* Imaging Speaker 20: Zhujun Wang (ShanghaiTech University)
	Molecular Reaction Dynamics at the Air-Water Interface Speaker 21: Xinxing Zhang (Nankai University)

Lecture 1：Construction of Zigzag Hydrocarbon Belts – An Organic Chemist’s Perspective on Carbon Nanostructures

Speaker：Prof. Meixiang Wang （王梅祥 教授）

Tsinghua University (清华大学)

Abstract: Zigzag hydrocarbon belts such as belt[n]arenes or [n]cyclacenes and their partially hydrogenated analogs (Figure 1) have been fascinating chemists and materials scientists for decades because of their aesthetically appealing molecular structures, tantalizing physical properties and intriguing chemical reactivities. They are unique and useful macrocyclic hosts in supramolecular chemistry. They may also serve as templates or seeds to grow structurally well-defined uniform zigzag carbon nanotubes. Despite synthetic effort in the past decades, the synthesis of zigzag hydrocarbon belts remains a great challenge. Very recently, we[1-3] have reported a general and straightforward fjord-stitching strategy to construct zigzag hydrocarbon belts from inexpensive and easily available resorcin[n]arenes. The method has been extended to the synthesis of edge-functionalized zigzag hydrocarbon belts and heteroatom-embedded zigzag hydrocarbon belts. Aromatization of octahydrobelt[8]arene with an access amount of DDQ led to the formation of a belt[8]arene-$(DDQ)_4$ adduct which underwent probably retro-Diels-Alder reaction, allowing the observation of the first fully conjugated zigzag hydrocarbon belt. In this talk, I will focus on the synthesis and structures of zigzag hydrocarbon belts. Perspectives on the strategies to isolate and characterize the fully conjugated belt[n]arenes and on the applications of zigzag hydrocarbon belts are also discussed.

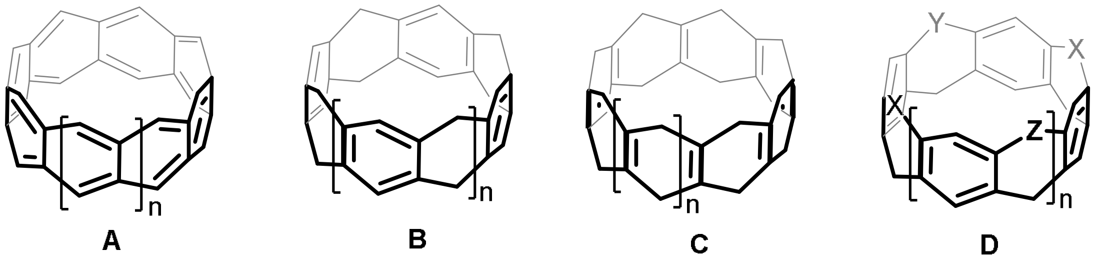


Figure 1. Structures of zigzag hydrocarbon nanobelts

References

1. (a) Q. Zhang, Y.-E. Zhang, S. Tong, M.-X. Wang, *J. Am. Chem. Soc.* **2020**, *142*, 1196-1199. (b) T.-H. Shi, Q.-H. Guo, S. Tong, M.-X. Wang, *J. Am. Chem. Soc.* **2020**, *142*, 4576-4580. (c) T.-H. Shi, S. Tong, M.-X. Wang, *Angew. Chem. Int. Ed.* **2020**, *59*, 7700-7705. (d) Y. Zhang, S. Tong, M.-X. Wang, *Angew. Chem. Int. Ed.* **2020**, *59*, 18151-18155. (e) M.-L. Tan, Q.-H. Guo, X.-Y. Wang, T.-H. Shi, Q. Zhang, S.-K. Hou, S. Tong, J. You, M.-X. Wang, *Angew. Chem. Int. Ed.* **2020**, *59*, 23649-23658.
2. For an overview on zigzag hydrocarbon belts, see, T.-H. Shi, M.-X. Wang, *CCS Chem.* **2020**, *2*, 916-931.
3. For a review on zigzag and other type aromatic molecular belts, see, Q.-H. Guo, Y. Qiu, M.-X. Wang, J. F. Stoddart, *Nat. Chem.* **2021**, 13, 402-419.

Prof. Meixiang Wang graduated from Fudan University (1983). After spending 3 years in Beijing General Research Institute of Non-ferrous Metals as a research associate, he joined Institute of Chemistry, Chinese Academy of Sciences (ICCAS) at Beijing and obtained his master degree (1989) and PhD (1992) under the supervision of Prof. Zhi-Tang Huang. He then worked at ICCAS ranking from assistant professor, associate professor to full professor. He has joined Tsinghua University since the May of 2009. His research interest includes macrocyclic and supramolecular chemistry of heteracalixaromatics, coronarenes and zigzag hydrocarbon belts, anion-π non-covalent bond interactions, high valent organocopper chemistry, catalytic and biocatalytic enantioselective reactions and applications.

Lecture 2：Understanding Carrier Transfer Across Interfaces in Metal Halide Perovskites

Speaker：Prof. Juan-Pablo Correa-Baena *Online*

Georgia Institute of Technology, USA

Abstract: Perovskite solar cells promise to yield efficiencies beyond 30% by further improving the quality of the materials and devices. Electronic defect passivation and suppression of detrimental charge-carrier recombination at the different device interfaces has been used as a strategy to achieve high performance perovskite solar cells. However, the mechanisms that allow for carriers to be transferred across these interfaces are still unknown. In this presentation, Prof. Juan-Pablo Correa-Baena will discuss the role of crystal surface structural defects on optoelectronic properties of lead halide perovskites through synchrotron-based techniques. The importance of interfaces and their contribution to detrimental recombination will also be discussed. As a result of these contributions to better understanding 2D and 3D defects, the perovskite solar cell field has been able to improve device performance. Albeit the rapid improvements in performance, there is still a need to understand how these defects affect long term structural stability and thus optoelectronic performance over the long term.

Juan-Pablo Correa-Baena is an Assistant Professor and the Goizueta Junior Faculty Rotating Chair in the School of Materials Science and Engineering at the Georgia Institute of Technology in Atlanta, USA. His group focuses on understanding and control of electronic dynamics at the nanoscale of low-cost semiconductors, such as halide perovskites and other materials, for solar cell and light emitting diode applications. Juan-Pablo’s group works on advanced deposition techniques, with emphasis on low-cost equipment and high throughput, as well as advanced characterization methods that include synchrotron-based mapping and imaging approaches with nanoscale resolution.

Juan-Pablo has published over 100 peer-reviewed papers in materials science for optoelectronic devices and some of the most impactful work in perovskite solar cell research, in the journals *Nature, Science*, *Energy and Environmental Science, Advanced Materials,* and *Nature Energy,* among others. Juan-Pablo received his PhD from the University of Connecticut, where he studied metal oxide aerogels as porous conductive electrodes for dye-sensitized solar cells, funded by two National Science Foundation fellowships. His work as a postdoctoral fellow in the group of Prof. Michael Grätzel at the Ecole Polytechnique Fédérale de Lausanne focused on understanding of fundamental questions regarding band offsets at interfaces in perovskite solar cells. He was awarded the highly competitive Department of Energy EERE fellowship to conduct work at MIT, where he helped shed light onto minority phase formation and elemental distribution in complex, multi-element halide perovskites. His work at MIT lead to a first-author publication in the journal *Science*. His contributions have helped boost the efficiencies of perovskite solar cells above 25%, achieved by MIT researchers. His work has been cited over 20,000 times (h-index of 50) making him a top cited researcher as recognized by the Web of Science Group**,** *Highly Cited Researchers-cross-field* (2019) and *Chemistry* (2020)*,* and Nature Index**,** *Leading early career researcher in materials science* (2019).

Juan-Pablo has been a Guest Editor for a special issue on photovoltaics in the journal *PLOS One*, and is a board member of the materials science and engineering journal *Matter,* from Cell Press. He is a regular reviewer for top journals, including *Science*, *Nature*, and *Energy and Environmental Science*. He has also been an organizer for several MRS symposia that deal with solar cell research. His contributions to society at large include disseminating his work via TV, where he has given several interviews about his research, and social media, where he has a strong and growing following on Twitter.

Lecture 3：Synthesis and Imbalanced C–H Activation Reactivity of a Terminal Co Oxo Complex

Speaker：Prof. John Anderson *Online*

University of Chicago, USA

Abstract: Transition metal oxo complexes, particularly those of later transition metals, have been cited as important intermediates in processes such as C-H hydroxylation and oxygen evolution. In general, however, these species are highly reactive and difficult to isolate and study. In this talk I will present our laboratory’s efforts at isolating and studying late transition metal oxo complexes. We have found that use of pseudo-tetrahedral geometries enables the isolation of an unusual terminal Co-oxo complex. The reactivity of this species towards C-H activation is markedly different than that observed for the majority of other systems and provides experimental evidence for a new mechanistic scenario arising from imbalanced thermodynamic driving forces. We show that far from being unique to this system, such “imbalanced” transition state effects are general and are also fully compatible with quantum mechanical nonadiabatic CPET reactions.

Prof. John Anderson was born in Downers Grove, a suburb about 40 minutes west of Chicago. He acquired his interest in chemistry at an early age from his grandmother, who was a chemist at Abbott Laboratories in North Chicago. Seeking to further his study of science, John matriculated at the University of Chicago. Once there, John quickly joined the laboratory of Professor Greg Hillhouse. It was in the three years that John spent in Greg's lab that he found his love for inorganic chemistry. During this time, John focused on researching phosphine complexes of Ni, specifically with respect to their reactivity with small molecules such as carbon dioxide and carbon disulfide.

After graduating John began his graduate studies in Boston at MIT in the group of Professor Jonas Peters. His time in Boston was to be short-lived however, as the Peters group moved to the California Institute of Technology in sunny Pasadena, CA quickly thereafter. John also made the move and received his Ph.D. from Caltech. John's thesis centered around a discrete Fe complex that mediates catalytic nitrogen fixation to ammonia.

After finishing his thesis, John came to Northwestern to work in the laboratory of Dave Harris. During this time, John has focused on materials, particularly metal organic frameworks. A central theme is the ability to stabilize reactive species, such as low coordinate dioxygen adducts, within metal organic frameworks thus allowing their characterization and study.

In his independent career, John and the Anderson group have been interested in linking the physical properties of transition metal centers, particularly their spin and radical character, to reactivity and bulk properties.

Lecture 4：Combining Synthetic Chemistry and Biology for Streamlining Access to Complex Molecules

Speaker：Prof. Hans Renata *Online*

The Scripps Research Institute, USA

Abstract: By virtue of their unrivaled selectivity profiles, enzymes possess remarkable potential to address unsolved challenges in chemical synthesis. The realization of this potential, however, has only recently gained traction. Recent advances in enzyme engineering and genome mining have provided a powerful platform for identifying and optimizing enzymatic transformations for synthetic applications and allowed us to begin formulating novel synthetic strategies and disconnections. This talk will describe our recent efforts in developing a new design language in chemical synthesis that centers on the incorporation of biocatalytic approaches in contemporary synthetic logic. Case studies will focus on the use of this platform in the chemoenzymatic syntheses of complex natural products and also highlight how this platform could serve as a starting point to enable further biological and medicinal chemistry discoveries.

Prof. Hans Renata received his B.A. degree from Columbia University in 2008 and earned his Ph.D. from The Scripps Research Institute in 2013 under the guidance of Prof. Phil S. Baran. After postdoctoral studies with Prof. Frances H. Arnold at Caltech, he began his independent career at The Scripps Research Institute in 2016. His research focuses on synthetic and biosynthetic studies of natural products and biocatalytic reaction developments.

Lecture 5：为合成科学插上化学与生物两只翅膀

Speaker：Prof. Xiaoguang Lei（雷晓光 教授）

Peking University （北京大学）

Abstract: 化学合成一直以来是推动生物医学研究和创新药物开发的重要基础。但是，目前对于具有重要生物活性和复杂结构的有机分子，特别是天然产物分子的合成效率还远远没有达到理想效果。与化学合成相对应的基于酶催化反应的生物合成方法在底物的高选择性和高催化效率等方面具有一定优势。但是，在很多情况下，酶法合成的底物广泛性和所能催化的化学转化类型还有待提高。因此，基于酶催化的生物合成方法与传统化学合成方法具有良好的互补性。在此次报告中，我将以“化学酶法推动创新药物研发”为核心讲演内容，提出实现复杂有机分子的“完美合成”这一关键科学问题，通过有效地整合化学合成与生物酶催化合成，取长补短、充分发挥各自的最大优势，实现“原子经济性”、“操作流程经济性”和“氧化/还原经济性”，从而帮助实现复杂天然产物、药物分子的高效、精准制备。

雷晓光，北京大学化学与分子工程学院教授，北大-清华生命科学联合研究中心高级研究员，深圳湾实验室肿瘤研究所资深研究员。2001 年本科毕业于北京大学化学学院，2006 年获得美国波士顿大学有机合成化学博士学位，2006-2008 年在美国哥伦比亚大学从事生物有机化学博士后研究，2008 年底全职回国，曾任北京生命科学研究所高级研究员，2014 年全职加入北京大学化学学院。独立工作以来，在复杂天然产物全合成，活性小分子探针导向的化学生物学，生物合成与酶催化，以及创新药物研究领域取得了一系列具有原创性的科学发现；目前在 *Cell, Nature, Science, Nature Chemistry, Nature Chemical Biology* 等期刊上发表论文 100 余篇，并获得了 20 余项创新药物发明专利授权；荣获了国家杰出青年基金、科技部 973、863 首席科学家、万人计划等学术荣誉；还获得了国际四面体青年科学家奖，国际化学生物学协会青年科学家奖，以色列 David Ginsburg Award，中国化学会-巴斯夫青年知识创新奖、维善天然产物合成奖、青年化学奖，中国药学会施维雅药物化学家奖等 20 项国内外学术奖励；目前担任 BMC 杂志执行主编。

Lecture 6：Chemical Proteomic Profiling of Functional Modifications by Reactive Metabolites

Speaker：Prof. Chu Wang（王初教授）

Peking University （北京大学）

Abstract: Genome sequencing projects have revolutionized our view of the complexity of prokaryotic and eukaryotic proteomes, however, we are also left with a daunting challenge of functionally annotating these large number of predicted proteins. Chemical proteomic methods, such as activity-based protein profiling (ABPP), have been developed aiming at systematically discovering new functional targets directly from native proteomes. In this talk, I will present recent progresses from my laboratory which combine ABPP-based chemical proteomic, biochemical and computational strategies to uncover functional sites of post-translational modifications by reactive metabolites in proteomes.

Prof. Chu Wang received his bachelor degree in biology from University of Science and Technology of China (USTC) in 2001. He got his Ph.D. in 2007 from University of Washington under the guidance of Professor David Baker, training in the area of computational protein structural prediction and design. He then worked as a postdoctoral fellow with Professor Benjamin Cravatt at The Scripps Research Institute, Lo Jolla, and developed multiple chemical proteomic methods to profile reactive cysteines and modifications in proteomes. In 2014, he joined College of Chemistry and Molecular Engineering, Peking University as a tenure-track assistant professor of Chemical Biology and was promoted to the full professorship in 2020. Currently he is also appointed as a Principal Investigator at the PKU Synthetic and Functional Biomolecules Center (SFBC) and the PKU-Tsinghua Center for Life Sciences (CLS). His research interest is to develop chemical and computational proteomics methods to enable quantitative profiling of functional enzymes, protein post-translational modifications as well as protein-ligand interactions in proteomes. He received the “ICBS Young Chemical Biologist Award” from International Chemical Biology Society in 2018 and the “Distinguished Young Scholars Award” from National Natural Science Foundation of China in 2019.

Lecture 7：*Exo*-Selective Diels–Alder Reactions Enabled by a Bispyrrolidine Diboronate

Speaker：Prof. Zhen Yang（杨震 教授）

Peking University（北京大学）

Abstract: Catalytic asymmetric Diels−Alder reaction is one of the most useful reactions in organic chemistry as it can potentially generate a six-membered ring with up to four chiral centers, thus attracting continues attentions. It is a great challenge to achieve only one product out of eight possible stereoisomers, which is often considered the task of an enzyme, causing tremendous efforts in searching for Diels-Alderases. Here we report a novel bispyrrolidine diboronate compound which is derived from the reaction of two molecules of oxazaborolidine with one molecule of water. Upon activation, it effectively catalyzes (0.4-5 mol % loading) the Diels–Alder reaction between a variety of mono- and di-carbonyl activated dienophiles and dienes with better than 20:1 regioselectivity, up to >99:1 enantioselectivity, and better than 20:1 *exo*/*endo* selectivity. Based on theoretical studies a model is proposed to rationalize the above observations. Due to the dimeric nature of the catalyst, a cavity is formed as the catalytic center. The dienophile substrate binds in an S-*cis* conformation, and the diene has to take a Si *exo* approach towards the dienophile. This reaction opens a wide window for the synthesis of a large number of natural products which are otherwise difficult to synthesize using existing methods.

Prof. Zhen Yang studied medicinal chemistry at Shenyang College of Pharmacy and earned a Ph.D. at The Chinese University of Hong Kong in 1992 under the guidance of Professor H. N. C. Wong. He carried out postdoctoral research on natural product synthesis with Professor K. C. Nicolaou at The Scripps Research Institute in La Jolla, CA, USA and joined its faculty in 1995. In 1998, he moved to the Institute of Chemistry and Cell Biology at Harvard Medical School as an institute fellow before returning to China as a professor at Peking University in 2001. Since 2008, he has served as the founding Dean of the School of Chemical Biology and Biotechnology of Peking University of Shenzhen Graduate School. He is recognized for his work in organic synthesis, natural product total synthesis and synthetic methodology development.

Lecture 8：含氟复杂分子的合成研究

Speaker：Prof. Pingping Tang（汤平平 教授）

Nankai University（南开大学）

Abstract: 由于氟原子特殊的性质，含氟有机物在医药，农药，医学检测，材料等领域有着广泛的应用。其中，三氟甲氧基由于具有强吸电子性和高酯溶性，在医药，农药等领域引起了合成化学家广泛的关注。但是，由于传统的三氟甲氧基化试剂较少，且毒性大，操作困难。另外，三氟甲氧基负离子不稳定，容易分解成氟负离子和氟光气分子，导致三氟甲氧基化合物的高效合成具有极大的挑战性，一直是氟化学领域的难点。我们发展了一类全新的三氟甲氧基化试剂——三氟甲基苯磺酸酯（TFMS），首次实现了银催化烯烃的不对称溴代三氟甲氧基化反应。该三氟甲氧基化试剂制备简单，并且具有良好的稳定性，反应活性好等优点。基于新型的三氟甲氧基试剂（TFMS），我们进一步发展了一系列温和条件下的三氟甲氧基化新方法。该系列方法可以直接实现复杂分子的后期三氟甲氧基化，为复杂分子的后期三氟甲氧基化提供了新方法。

汤平平，南开大学教授、博士生导师。2002 年本科毕业于南开大学，2007 年博士毕业于中国科学院上海有机化学研究所，师从俞飚研究员。2008 年 8 月-2012 年，在哈佛大学从事博士后研究，师从 Tobias Ritter 教授。2012 年 9 月加入南开大学任特聘研究员、独立课题组长，2018 年 9 月晋升教授。曾获中国化学会青年化学奖、Thieme Chemistry Journals Award、中国均相催化青年奖、国家基金委杰出青年基金（2019）等奖项和资助。研究兴趣：氟化学研究和天然产物全合成研究。迄今已在 *Nat Chem*、*Nat Commun.*、*JACS*、*ACIE* 等杂志发表学术论文 50 余篇。

Lecture 9：有机功能染料与产品工程

Speaker：Prof. Weihong Zhu（朱为宏 教授）

East China University of Science and Technology（华东理工大学）

Abstract: 精细化工作为化工产品产业链的重要制高点，面临深度加工、应用创新、突破“卡脖子”瓶颈。以有机染料为例，聚焦分子化学工程，源头性能提升到产业化应用。基于强吸电子受体，揭示能级调控、强化电荷分离机制关注分子设计源头创新，发展染料功能性、稳定性策略，提升功能染料产业化应用及产品工程，寻求精细化工与传品工程高地。

朱为宏，现任华东理工大学副校长、精细化工研究所所长。国家杰出青年基金获得者（2013 年），曾入选长江学者特聘教授（2015 年）、中组部万人计划科技创新领军人才（2016 年）、国务院特殊津贴（2018 年）、教育部新世纪优秀人才（2007 年）、上海市学术带头人（2015 年）。

1992 年 7 月毕业于南京师范大学化学系，1995 年 7 月在南开大学化学系获有机化学硕士学位，1999 年 7 月在华东理工大学获应用化学博士学位，2001 年 10 月至 2003 年 4 月，日本筑波国立产业技术综合研究院（AIST）纳米研究所博士后研究，2004 年 7 月至 2005 年 3 月，日本筑波大学先进学际研究中心（TARA Center）外国人研究员（高级访问学者）。

目前主要从事化学产品工程研究，方向染料功能化及产品化，包括荧光染料、光致变色染料、敏化染料。迄今已发表 SCI 论文 310 余篇，共被 SCI 引用 1.8 万余次， H 指数为 74。申请中国发明专利 36 项，其中 28 项已授权，曾获国家自然科学奖二等奖两项（2019 年第一完成人；2007 年第三完成人）、上海市自然科学奖一等奖两项（2017 年第一完成人；2006 年第三完成人）、上海市科技进步奖一等奖（2020）、上海市牡丹奖等。入选 2018、2020 年度科睿唯安化学领域“高被引科学家“（Highly Cited Researchers）。

目前担任中国化工学会染料专委会副主任委员、中国化工学会精细化工专业委员会常务委员、中国化学会光化学专委会副主任委员、中国感光学会第八届理事会常务理事，并担任《*Green Chemical Engineering*》副主编、《过程工程学报》副主编、《影像科学与光化学》常务副主编、*Science China Chemistry* 编委、*ACS Applied Bio Materials* (ACS-ABM) 编委、*Dyes and Pigments* 编委、*Green Energy and Environment* 编委等。

Lecture 10：Nickel-Mediated Radical Pathways and Applications in *C*-Glycosylation

Speaker：Prof. Tianning Diao（刁天宁 教授） *Online*

New York University, USA

Abstract: Reactions involving organic radical intermediates have been traditionally regarded as overly reactive and unselective. Nickel complexes can reversibly coordinate to radicals, and thus modulate the reactivity and control the selectivity of reactions involving radical intermediates. We probe fundamental questions, such as "how do nickel complexes initiate radical formation from various precursors", "how do radicals interact with nickel complexes", and "How do ligands serve to stabilize open-shell intermediates and facilitate catalytic reactions?" Mechanistic insight has informed us in the development of a new glycosyl radical precursor for the syntheses of *C*-glycosides, including nucleoside analogues, crucial for drug discovery and chemical biology studies.

Prof. Tianning Diao is an Associate Professor of Chemistry. She received her Ph.D. in Chemistry from the University of Wisconsin–Madison in 2012 and conducted postdoctoral research at Princeton University from 2012 to 2014. Since joining the faculty at NYU in 2014, her research has focused on understanding the mechanism of nickel-catalyzed cross-coupling reactions and developing new methods to address challenges in organic synthesis of sustainable energy conversion. Diao is a recipient of the NSF-CAREER award (2016), Sloan Research Fellowship (2018) Chinese-American Chemistry Professors Association Distinguished Junior Faculty Award (2018), Organometallics Distinguished Author Award (2018), Camille-Dreyfus Teacher-Scholar Award (2019), and Thieme Chemistry Journal Award (2019).

Lecture 11：手性 Lewis 碱和过渡金属协同不对称催化

Speaker：Prof. Liuzhu Gong（龚流柱 教授）

University of Science and Technology of China （中国科学技术大学）

Abstract: 有机小分子和金属联合催化剂可同时或连续活化多个化学键并使其有序重组，因此能够发展单一催化剂难以实现的反应。2001 年我们首次报道了手性有机小分子和金属联合催化的不对称反应，突破了在不对称金属催化中依靠手性配体控制立体选择性的传统观念。近年来，我们先后发展了手性布朗斯特酸/金属和手性双功能有机小分子/金属等联合催化剂，实现了一系列单一催化剂体系难以完成的不对称有机化学反应。本次报告将主要介绍我们最近在 Lewis 碱和过渡金属联合催化方面取得的进展。

龚流柱，1970 年 10 月出生，博士，教授。1993 年毕业于河南师范大学化学系，1996 年在中国科学院成都有机化学研究所获硕士学位，2000 在中国科学院化学研究所获理学博士学位。2000-2005 年在中国科学院成都有机化学研究所工作，先后任助理研究员、副研究员和研究员。2006 年 1 月至今任中国科学技术大学教授。2003 年获得国家杰出青年基金资助，2007 年被聘为教育部长江学者特聘教授，2016 年被评为国家“万人计划”领军人才。主要从事不对称催化和天然产物全合成研究；与合作者发现了氨基酸酰胺能高立体选择性地催化不对称有机化学反应，提出了“烯胺-双氢键”活化模型；提出了“手性有机小分子/金属”协同催化的策略，发展了新型催化模式。以通讯作者在国际学术刊物发表论文 170 多篇。先后获中国化学会有机化学专业委员会“有机合成创造奖”（2005），中国化学会-巴斯夫公司青年知识创新奖（2009），中国化学会“青年手性化学奖”（2012），以第一完成人获得安徽省科学技术奖一等奖（2012）和国家自然科学奖二等奖（2013）各一项。

Lecture 12：Discovery and Biosynthesis of Marine Actinobacteria-Derived Polycyclic Natural Products

Speaker：Prof. Changsheng Zhang（张长生 研究员）

South China Sea Institute of Oceanology（中科院南海海洋研究所）

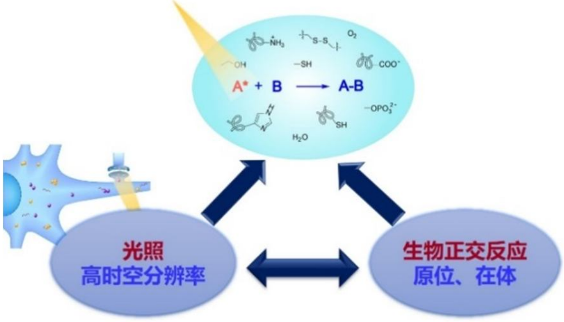
Abstract: 海洋微生物日益成为发现具有显著生物活性和新骨架天然产物的重要资源。我们多年的研究表明，海洋微生物不但具有丰富的物种多样性，而且能够生产多种多样的具有多环结构的新颖天然产物，如具有螺环结构的生物碱等。另外，我们还发现，通过基因组挖掘以及启动子工程和调控子操纵等手段，可以激活沉默基因簇，进一步增强海洋微生物多环天然产物的结构多样性。生物合成研究表明，多环的形成具有不同的化学和酶学机制，如通过氧化级联反应形成厦霉素中的 5 元并环，而斑鸠霉素中的大环多环内酰胺则是通过一系列的还原成环反应形成，一些多环产物甚至还可以通过非酶催化的反应来构建。本文汇报了我们课题组近期在海洋微生物多环天然产物的发现及其成环机制方面所取得的一些进展。

张长生，中国科学院南海海洋研究所，研究员，副所长，国家基金委杰出青年基金获得者，英国皇家化学学会会士。主要从事海洋微生物天然产物的发现及其合成生物学研究，发现了一系列具有自主知识产权、具有抗感染、抗肿瘤和免疫抑制活性的新骨架海洋微生物天然产物，阐明了十余种海洋放线菌天然产物生物合成的独特化学机理和酶学机制，将合成生物学引入海洋微生物进行实践和创新，在 *Science*、*Nat Commun*、*JACS*、*Angew Chem*、*Chem Sci* 等主流期刊发表论文 140 余篇。担任 *Natural Product Reports*、*Molecules* 编委。获国务院政府特殊津贴、国家百千万人才工程、“万人计划”、广东特支计划杰出人才（南粤百杰）等荣誉。

Lecture 13：时空分辨的生物正交反应及分子探针

Speaker：Prof. Yan Zhang（张艳 教授）
Nanjing University（南京大学）

Abstract: 借助光照激发作为刺激源，结合可受光调控的分子工具，可实现对生物体系内的分子事件进行时间空间分辨的扰动，是研究复杂动态生命体系中分子事件的独特方法。生物正交反应则使得利用外源探针对复杂生物体系进行原位、在体的探索成为可能。如果能够用光来驱动生物正交反应，则有望开发出丰富的高时空分辨率的分子工具，为单细胞甚至亚细胞水平的动态分子事件的解析提供独特的化学生物学方法和技术。然而开发新的生物正交反应极具挑战性。2000 年报导的第一例生物正交反应是化学生物学领域的里程碑事件，但在随后的 20 年里开发出的新生物正交反应极少，生物正交工具箱里的分子工具非常匮乏，其中尤其缺乏具有时空分辨率的生物正交分子工具。用光驱动生物正交反应是实现时空分辨的可能途径，但光反应中的高能激发态和高活性中间体在复杂生物体系中如何实现可控的专一反应，这是开发光驱动生物正交反应必须挑战的一大难题。在此报告中，我将主要介绍我们结合不同策略开发生物正交反应的最新进展，包括可见光驱动的生物正交反应及无需外界刺激及张力促进的生物正交环加成反应的发现。结合生物正交反应和功能分子如核酸等，我们还发展了对其进行化学修饰以实现基于光成键反应的时空分辨调控等。



张艳，1997 年本科毕业于吉林大学，2002 年博士毕业于南京大学，2002-2004 年在香港科技大学化学系做博士后，2004 年至 2006 年在斯坦福大学医学院做博士后。2006 年 9 月起任南京大学化学化工学院教授，建立独立课题组开展光化学与化学生物学交叉的研究，致力于开发光诱导的生物正交反应及其在化学生物学研究中的新应用。2014 年入选中组部青年拔尖人才。2016 年起任南京大学化学化工学院副院长，2018 年起兼任南京大学化学化工学院化学生物学学科主任。

Lecture 14：无机磷材料的化学生物学研究

Speaker：Prof. Jing Zhao（赵劲 教授） *Online*

Nanjing University（南京大学）

Abstract: 在众多的无机纳米材料中，二维磷基材料引起了广泛的关注。黑磷材料在生物医学等众多领域都具有潜在的应用价值。我们从黑磷材料入手，首先对黑磷材料的蛋白冠进行了蛋白质鉴定及生信分析，研究了黑磷材料免疫治疗功能的机理；同时，我们发现了氧化黑磷纳米材料的骨靶向治疗功能，为进一步设计新的纳米药物提供了新的思路。最后，我们研究了一类广泛存在于生物系统各种细胞中的天然磷基材料——多聚磷酸盐 PolyP，通过解析它介导的蛋白质相分离，探索了其可能的生物学功能和产业化前景。

赵劲，南京大学化学化工学院教授，主要从事生物无机化学研究工作。1998 年本科毕业于南京大学化学系，之后在耶鲁大学攻读博士学位。2005 年至 2006 年于加州大学伯克利分校从事博士后研究。2006 年至 2007 年于芝加哥大学从事博士后研究。2007 年至 2008 年在罗门哈斯公司研发部工作。2008 年 6 月加入南京大学任教授、博士生导师。2009 年-2014 年担任北京大学深圳研究生院化学生物学与生物技术学院副院长、博士生导师。2020 年获得国家自然科学基金委员会“杰出青年基金”支持。

Lecture 15：Molecular Materials Property Prediction: Mechanism and Computational Methods

Speaker：Prof. Zhigang Shuai（帅志刚 教授）

Tsinghua University（清华大学）

Abstract: 今日化学的研究重点已经由结构转向功能。我们面向分子固体材料的功能计算与模拟发展了若干计算方法与程序。我们将介绍我们所发展计算有机发光和电荷输运性质的计算方法，包括我们提出的核隧穿驱动电荷传输的模型。最后，我们介绍最近提出了三线态激子与光子耦合可以提高逆系间穿越速率的新机制[1]。

[1] Qi Ou, Yihan Shao, Zhigang Shuai*, “Enhanced reverse intersystem crossing promoted by triplet exciton-photon coupling”, *J Am Chem Soc* **2021** (accepted).

帅志刚，清华大学化学系长江学者特聘教授，国家杰出青年基金获得者，中国化学会副理事长。1983 年中山大学物理系获学士学位，1989 年复旦大学物理系获博士学位。1990 起，在比利时蒙斯大学从事研究工作 11 年。2000 年入选科学院百人计划，加入中科院化学所工作。2008 年调入清华大学。长期从事理论化学研究，发展了电子激发态的结构与过程计算方法，发展了电子相关和电子-振动耦合的密度矩阵重整化群理论，开发了分子功能材料发光效率与载流子迁移率的计算程序 MOMAP，目前已经实现了商业化应用。发表 420 余篇论文，被引用 22000 余次(h 因子=81)。2008 年当选为国际量子分子科学院院士，并于 2018 年当选为副院长。2011 年，当选欧洲科学院(Academia Europaea) 外籍院士。2012 年获中国化学会阿克苏-诺贝尔化学科学奖。2013 年，当选为比利时皇家科学院外籍院士。2017 年，当选为世界理论与计算化学家协会(WATOC)科学理事。2018 年，获法国化学会法-中化学讲座奖。荣获 2020 年北京市自然科学奖一等奖（排名第一）。2021 年，当选为国际纯粹与应用化学联合会(IUPAC)执行局常务委员。

Lecture 16：Visualizing a Single Molecule at the Single-Bond Limit

Speaker：Prof. Yi Luo（罗毅 教授）

University of Science and Technology of China（中国科学技术大学）

Abstract: Light has been widely used to characterize molecular structure and properties. However, the spatial resolution of light-based techniques is often in the region of hundred nanometers because of the intrinsic diffraction limit, which is much larger than the size of the molecule. The generation of nanocavity plasmon has made it possible to break the diffraction limit, enabling to visualize a molecule at sub-nanometer level. Here, I will briefly introduce our progresses in developing chemical imaging techniques for single molecules in recent years by addressing three questions, namely, (1) how can a single molecule image be acquired? (2) What does the image tell? (3) How could the images be utilized to solve chemical problems?

罗毅，教授，博士生导师，现任合肥微尺度物质科学国家研究中心主任，中科院量子创新研究院副院长，国家特聘专家，国家杰出青年基金获得者。 1985 年在华中工学院获得工学学位，1985-1989 年在中科院上海光机所硕博连读，1996 年在瑞典林雪平大学获计算物理博士学位，曾在瑞典斯德哥尔摩大学任助理教授，瑞典皇家理工学院任副教授、教授、兼职教授。长期从事化学物理研究，系统发展了局域光场与物质相互作用理论和计算方法，发展了可视化重构分子化学结构的扫描拉曼埃分辨显微术（SRP），发展了局域场驱动的非线性电子散射谱 (NESS)技术。获得 2010 年瑞典皇家科学院“Goran Gustafsson”化学奖，2014 年作为主要完成人之一获中国科学院“杰出科技成就集体奖”。在国际重要学术期刊发表论文 500 余篇，入选 2020 年科睿唯安“高被引科学家”名单。

Lecture 17：多孔芳香骨架材料-PAFs

Speaker：Prof. Guangshan Zhu（朱广山 教授）
Northeast Normal University（东北师范大学）

Abstract: 目前，多孔芳香材料（PAFs）的研究已成为多孔材料家族的一个研究热点。多孔芳香骨架材料具有稳定性高、比表面积大、孔容大、可修饰性强等优势，在气体储存和分离、传感、催化、光电等展现了优良的性能。[1, 2]为了获得具有特定结构和可调控性质的多孔芳香骨架材料，选择合适的结构基元和有效的偶联反应类型具有非常重要的意义。在计算机设计模拟的帮助下，我们设计、合成了一系列多孔芳香骨架材料。通过研究其拓扑学结构，目标性地筛选确定合适的结构基元和高效的聚合反应，实现了高比表面积 PAFs 材料的设计合成。

基于合成与结构设计的工作基础，我们围绕多孔芳香骨架材料的结构可设计性这一特点，开发其多种先进功能的应用。具有阴离子中心、富电子炔键以及芳香性苯环等多种活性位点的 PAF 材料具有高达 2700 mg/g 的碘蒸气吸附量（Fig. 1a）。[3]通过在孔道内构建导电介质，利用电场作为驱动力实现 PAFs 材料高效海水提取铀（Fig. 1b）。[4]与具有催化活性的多酸阴离子结合，同时调控 PAFs 的孔隙率和多酸的催化活性（Fig. 1c）。[5]多孔芳香骨架材料将会在能源与环境相关的新型功能材料领域获得更多的突破性进展。

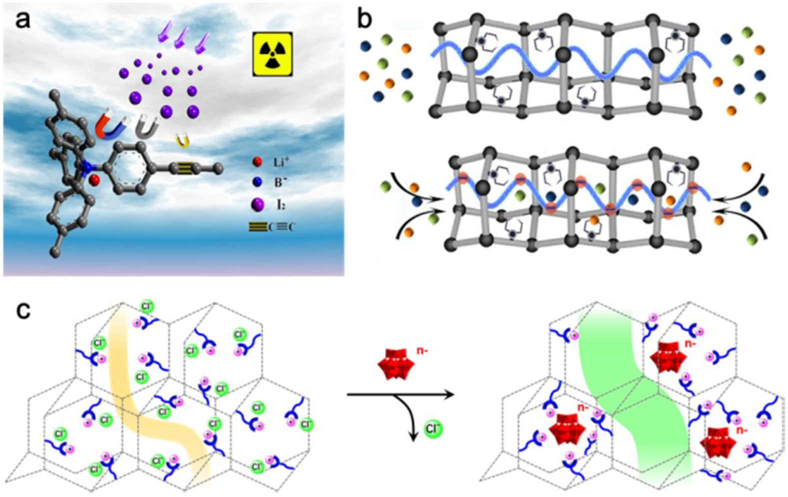


Fig. 1 PAF materials with (a) multiple active sites for iodine uptake, (b) combination of chemical chelating and electric field driven of uranium species and (c) porosity modulation via polymetalate anions.

关键词：多孔芳香骨架；结构设计；定向合成；气体分离；先进功能应用

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朱广山，国家杰出青年基金获得者，国家“万人计划”科技创新领军人才，博士生导师（“卢嘉锡优秀导师”获奖者）。东北师范大学教授，化学学院院长，民盟中央委员。主要从事多孔材料设计、合成与功能特性研究，开创多孔芳香骨架（PAFs）材料。近年来，在 *J. Am. Chem. Soc.*、*Angew. Chem. Int. Ed.*、*Nat. Commun.*、*Adv. Mater.*等国内外杂志发表研究论文 380 余篇，被引用 18000 余次，H-Index 为 73，出版英文专著 2 部，获得国内授权专利 20 余项。2014 年以来多次入选全球高被引科学家。多次应邀参加相关领域国际会议并担任分会主席。先后主持多项国家级重大和重点项目，主持国家自然科学基金（包括重点项目、重大国际合作项目、面上项目等）、省部级项目等 10 项以及 973 项目子课题 2 项。先后获得 2008 年国家自然科学二等奖（第二完成人）一项，2018 年吉林省科技进步一等奖（第一完成人）。

Lecture 18：*In Situ* Neutron Measurements in Materials Chemistry

Speaker：Prof. Howard Wang（王浩 教授）
University of Maryland, College Park, USA

Abstract: Large scientific research facilities such as synchrotron x-ray and neutron sources have enabled *in situ* measurement techniques for advancing the design, synthesis, processing and applications of materials. I will illustrate the application of *in situ* neutron measurements to those 4 aspects of materials research by using examples in the 4 focused fields of this WE Forum: (1) controlled synthesis and directed assembly of quantum dots and nanoparticles, (2) growth of lithium dendrites at the interface and in the bulk of solid electrolytes in rechargeable batteries, (3) enzymatic dephosphorylation of synthetic peptides and synergistic formation of hydrogels, and (4) tailored length and time scales in the bilayered-micelle to perforated-lamellae transition in phospholipid solutions. Opportunities and challenges of using neutron instruments in materials research will be discussed.

Prof. Howard Wang obtained his Bachelor of Science in Physics from the Peking University and Ph.D. in Materials Science and Engineering from the University of Pennsylvania in 1999. After postdoc research at NIST, he was an assistant professor at Michigan Technological Univ., an associate professor at the State University of New York, Binghamton, a research professor at the University of Maryland, College Park, and the founding director of the SLDF, the first deuteration facility in China. Wang has had extensive research experience in neutron techniques for studying soft matter, nanotechnology, electronics and batteries, and authored over 100 publications and 8 patents. Wang was a member of the Bohmische Physical Society, a recipient of the NSF Career Award, an Empire-State Professor at SUNY, and a NIST-ARRA Senior Research Fellow.

Lecture 19：Dynamics and Mechanism of Water Oxidation Catalysts

Speaker：Prof. Mårten S.G. Ahlquist *Online*

Royal Institute of Technology, Sweden

Abstract: Electrocatalytic water splitting is mainly limited by the water oxidation reaction, which in turn is limited by the formation of the first O-O bond. There are two main mechanisms for this reaction step, the water nuceleophilic attack on a metal oxo, and the radical coupling mechanism of two metal oxos. The former is typically slow but easily achieved, while the latter have been found to be extremely fast but much more challenging to control. A major challenge with the radical coupling mechanism is that it involves two metal centers, typically on two metal complexes, that need to interact without additional strain or electrostatic repulsion. Since our first publication on a dynamic study of the O-O bond formation of the highly efficient Ru(bda)L2 catalyst by Sun and co-workers, we have developed the technique to simulate key reaction steps for catalyst in highly complex environments. We will present simulations of catalyst diffusion, reaction steps, at water carbon interfaces, in presence of ions and high electric fields. Finally we will present a third mechanism for O-O bond formation, the oxide relay mechanism.

Prof. Mårten Ahlquist is a Professor and pro-prefect at the Department of Theoretical Chemistry & Biology at KTH Royal Institute of Technology in Stockholm Sweden. His work is focused on modelling of molecular catalysts, mainly for activation of strong bonds and small molecules, including C-H activation, water oxidation, electrochemical catalysis, CO_2 activation, and H_2 production. After his M.Sc. in 2004 at Lund University Sweden he moved to the Technical University of Denmark for his doctoral studies. He received his Ph.D. in 2007 for his work on palladium and copper catalyzed reactions involving alkynes. This work was supervised by Per-Ola Norrby in collaboration with experimental groups, including Nobel Laureate K. Barry Sharpless. In 2007 he began his postdoctoral studies at Caltech under the supervision of William A. Goddard III. The direction was still on metal catalyzed reactions, but now under more extreme conditions. The focus was on mechanistic studies of platinum catalyzed methane to methanol oxidation in fuming sulfuric acid. In 2009 he returned to Sweden and started his independent career at KTH in Stockholm. His current research is directed towards understanding molecular catalysts in complex and realistic environments, including solutions, at electrode-water interfaces, in metal-organic frameworks, and under the influence of electric fields.

Lecture 20：The Coalescence Behavior of Two-Dimensional Materials Revealed by Multiscale *In Situ* Imaging

Speaker：Dr. Zhujun Wang （王竹君 特聘研究员）
ShanghaiTech University（上海科技大学）

Abstract: Wafer-scale monocrystalline two-dimensional (2D) materials can theoretically be grown by seamless coalescence of individual domains into a large single crystal. Here we present a concise study of the coalescence behavior of crystalline 2D films using a combination of complementary *in situ* methods. Direct observation of overlayer growth from the atomic to the millimeter scale and under model- and industrially relevant growth conditions reveals the influence of the film–substrate interaction on the crystallinity of the 2D film. In the case of weakly interacting substrates, the coalescence behavior is dictated by the inherent growth kinetics of the 2D film. It is shown that the merging of coaligned domains leads to a distinct modification of the growth dynamics through the formation of fast-growing high-energy edges. The latter can be traced down to a reduced kink-creation energy at the interface between well-aligned domains. In the case of strongly interacting substrates, the lattice mismatch between film and substrate induces a pronounced moiré corrugation that determines the growth and coalescence behavior. It furthermore imposes additional criteria for seamless coalescence and determines the structure of grain boundaries. The experimental findings, obtained here for the case of graphene, are confirmed by theory-based growth simulations and can be generalized to other 2D materials that show 3- or 6-fold symmetry. Based on the gained understanding of the relation between film–substrate interaction, shape evolution, and coalescence behavior, conditions for seamless coalescence and, thus, for the optimization of large-scale production of monocrystalline 2D materials are established.

Keywords: multiscale *in situ* imaging, seamless coalescence 2D materials, complementary *in situ* methods, chemical vapor deposition, pressure gap

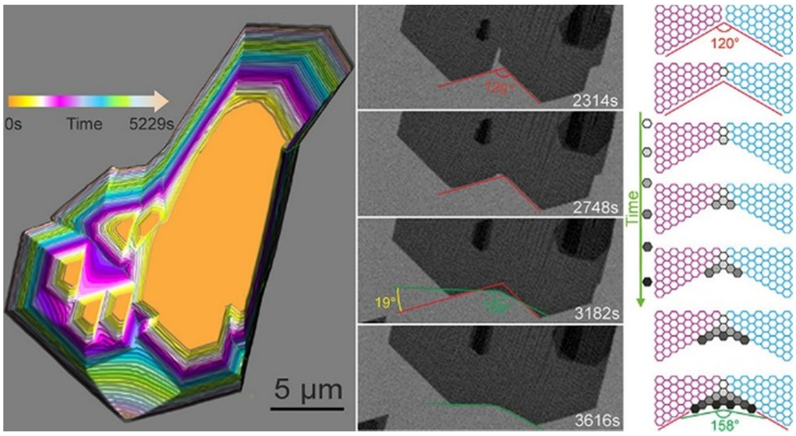


Fig. 1 Real-time *in situ* SEM shows coalescence behaviors of 2D material during CVD growth

Dr. Zhu-Jun Wang obtained his PhD in experimental physics at Fritz-Haber-Institute of MPG in 2015. After a senior scientist fellowship at ETH, since October 2020, Zhu-Jun is a group leader at, School of Physical Science and Technology, ShanghaiTech University. Dr. Zhu-Jun Wang is an expert on both electron microscopy and heterogeneous catalysis. He has successfully constructed the surface sensitive near-ambient-pressure *ex* scanning electron microscopy (SEM) during his doctoral research. With this technique, the detailed atomic-scale information obtained by *in-situ* transmission electron microscopy (TEM)/ scanning tunneling microscopy (STM) can be embedded within the global picture obtained at lower magnifications by *in-situ* SEM and subsequently correlated with the spectroscopic data from near ambient pressure *in-situ* X-ray photoelectron spectroscopy (NAP-XPS). This multi-scale approach enables to investigate the dynamic nature of catalyst during the ongoing work, bridges the pressure-gap, and links atomistic details to collective processes. One typical work is the analysis of surface dynamics, from the micrometer- to the atomic-scale, at well-controlled experimental environments to obtain a fundamental understanding of the mechanism of graphene and two dimensional (2D) materials growth on metal catalyst.

Lecture 21：Molecular Reaction Dynamics at the Air-Water Interface

Speaker：Dr. Xinxing Zhang （张新星 特聘研究员）

Nankai University（南开大学）

Abstract: Air-water interface is ubiquitous in nature, including the surface of ocean that takes up more than 70% of earth surface, the surface of cloud droplets, and the surface of human lungs and eyes (the tear film). Consequently, the chemistries that occur at the air-water interfaces are vital in understanding many environmental and biological processes.

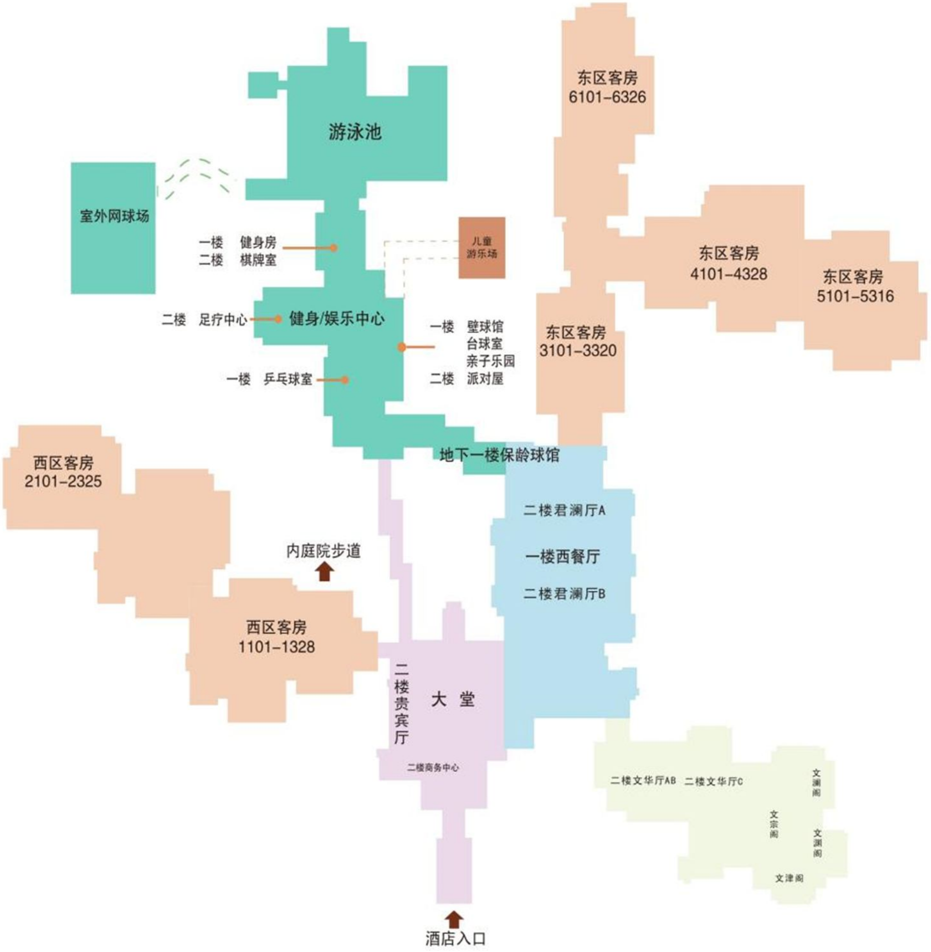
Sampling the ultra-thin air-water interface without any interference from the bulk is an obvious technical difficulty. To solve this problem, our lab utilized the unique field-induced droplet ionization mass spectrometry (FIDI-MS) methodology, which is capable of selectively sampling the monolayer of amphiphilic molecules that reside on the air-water interface in an “online” manner. By studying the oxidation chemistry initiated by hydroxyl radicals (OH), we have systematically elaborated many biologically relevant chemical processes that are highly influenced by the biophysical status of the monolayer.

More recently, our lab developed a new phased-array acoustic levitation (tweezers) technique, which is able to manipulate multiple particles simultaneously, and to deliver airborne, container-less chemical reactions. This technique has been combined with FIDI-MS to study the molecular-level mechanism of photodynamic therapy for cancer involving lipid oxidation.

张新星，南开大学化学学院研究员，主要研究方向为气液界面化学动力学和团簇分子反应动力学，迄今为止已发表 SCI 论文 72 篇，含第一或通讯作者论文 53 篇。回国独立工作以来，入选国家第十四批青年千人计划，在气液界面质谱学方向以南开大学为通讯单位发表论文 29 篇，其中包括 *Angew. Chem.* 7 篇，*JACS* 2 篇，*Nat. Commun.* 1 篇，*J. Phys. Chem. Lett.* 2 篇。获得了中国化学会第二届菁青化学新锐奖（本届全国共 5 名），美国质谱学会 ASMS 新兴科学家（Emerging Investigator）称号（本届全球共 11 名，2015 年该称号设立以来唯一中国大陆获得者），以及中国物理学会质谱专业委员会评选的 2021 年度质谱青年奖（全国唯一获奖人）。

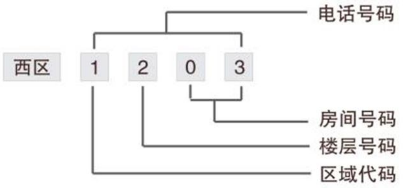
Venue（会议地址）

- **Hangzhou Narada Resort & Spa Liangzhu（杭州良渚君澜酒店）**
- **Address:** Liangzhu Cultural Village, Holiday Road, Yuhang District, Hangzhou City, Zhejiang Province（浙江省杭州市余杭区度假路良渚文化村内）
- **Tel:** 0571-56195202



房间号码说明：

示例：



上述编号所表示为：西区，1号楼，2楼，03号房，电话号码1203

注：区域代码和区域码对应如下：

西区对应区域代码为：1.2

东区对应区域代码为：3.4.5.6

Transportation（交通指南）

1. If you arrive at Hangzhou Xiaoshan International Airport by plane, you can directly take a taxi from the airport to the hotel. (The distance is about 58 kilometers, and the taxi fare is about 170 yuan).

2. If you arrive at Hangzhou East Railway Station by high-speed train:

   2.1 You can directly take a taxi from Hangzhou East Railway Station to the hotel (the distance is about 26 kilometers, the taxi fare is about 80 yuan).

   2.2 You can take Metro Line 1 to Fengqi Road, transfer to Line 2 to reach Dufu Village, and then take a taxi to the hotel (taxi fee is about 13 RMB).

1. 如果您乘飞机到达杭州萧山国际机场，您可以直接乘出租车从机场到酒店。(距离约 58 公里，出租车费约 170 元人民币)。

2. 如果您乘高速列车到达杭州东站：

   2.1 您直接可以乘出租车从杭州东站到酒店
   (距离约 26 公里，出租车费约 80 元人民币)。

   2.2 您可以乘地铁 1 号线到凤起路，换乘 2 号线到达杜甫村，然后乘出租车到酒店
   (出租车费用约 13 人民币)。

Accommodation（住宿推荐）

- **Hangzhou Narada Resort & Spa Liangzhu**

Room type	**Standard King Room/Standard Twin Room**
Price per night	**RMB 650**

Booking process:
Step 1: Call the hotel sales manager 13656653446
Step 2: Report the name of the meeting and enjoy the special price of the meeting
Step 3: The hotel will charge a part of the room rate as a deposit (cannot be cancelled after booking)
Step 4: Booking is successful!

- **SSAW Boutique Hotel** (It is 3.4km away from Liangzhu Junlan Resort, 8 minutes by taxi.)

Room type	**King Room/Twin Room**
Price per night	**RMB 375**

Booking process:
Step 1: Call the hotel reception +86-571-88777766
Step 2: Report the name of the meeting and enjoy the special price of the meeting
Step 3: The hotel will charge a part of the room rate as a deposit (cannot be cancelled after booking)
Step 4: Booking is successful!

- **Manju Prestige Hotel · Archaeological Ruins of Liangzhu City Hangzhou** (It is 9km away from Liangzhu Junlan Resort, 20 minutes by taxi.)

Room type	**Manju King Room/Manju Twin Room**
Price per night	**RMB 358**

Booking process:
Step 1: Call the hotel reception +86-571-88669777
Step 2: Report the name of the meeting and enjoy the special price of the meeting
Step 3: The hotel will charge a part of the room rate as a deposit (cannot be cancelled after booking)
Step 4: Booking is successful!

◆ 杭州良渚君澜酒店

房间类型	**标准大床房、标准双床房**
价 格	**650 元/晚**

预订流程：
第一步：致电酒店销售，手机号：13656653446
第二步：报会议名称即可享受酒店会议价
第三步：酒店会收取一部分房费作为押金（不可取消预订）
第四步：预定成功

◆ 杭州良韵君亭酒店 (距离良渚君澜度假酒店 3.4 公里，打车 8 分钟)

房间类型	**标准大床房、标准双床房**
价 格	**375 元/晚**

预订流程：
第一步：致电酒店前台，电话：+86-571-88777766
第二步：报会议名称即可享受酒店会议价
第三步：酒店会收取一部分房费作为押金（不可取消预订）
第四步：预定成功

◆ 开元曼居臻选·杭州良渚古城遗址店 (距离良渚君澜度假酒店 9 公里，打车 20 分钟)

房间类型	**曼居大床房、曼居双床房**
价 格	**358 元/晚**

预订流程：
第一步：致电酒店前台，电话：+86-571-88669777
第二步：报会议名称即可享受酒店会议价
第三步：酒店会收取一部分房费作为押金（不可取消预订）
第四步：预定成功

General Information（温馨提醒）

- **Registration**

Service Time： 13:00 – 20:00, 25th Oct.
08:00 – 20:00, 26th Oct.
08:00 – 17:00, 27th Oct.
Venue： Lobby, Hangzhou Narada Resort & Spa Liangzhu

- **Contact Information**

Ms. Qianqian CUI （+86 13738064493）

- **Emergency Phone Numbers**

119: Fire, Rescue
120: Hospital Services
110: Police

- **Weather Information**

It is autumn during October in Hangzhou, a pleasant season to visit the city. The temperature is typically between 13℃ to 21℃. It seems unlikely to rain, but just in case please take your umbrella with you.

- **会务服务台**

服务时间：10 月 25 日 13:00 – 20:00
10 月 26 日 08:00 – 20:00
10 月 27 日 08:00 – 17:00
地点：杭州良渚君澜酒店大堂

- **会务联系人**

崔倩倩（+86 13738064493）

- **紧急求救电话**

119 火警电话
120 紧急医疗求救电话
110 公安报警电话

- **天气信息**

会议时间时值金秋十月，杭州秋高气爽、金桂飘香。预计白天平均气温为 21 度，夜晚平均气温为 13 度。杭州常年多雨，友情提醒随身携带雨伞。

西湖大學
WESTLAKE UNIVERSITY

WORLD YOUNG
SCIENTIST SUMMIT
世界青年科学家峰会