Program

Thieme Organic Chemistry Symposia
China Roadshow 2024

The Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences

09:00-18:00 / 4 November 2024

The Lecture Hall, the 1st floor, Junmou Building
上海有机化学研究所君谋楼一楼报告厅

Thieme

中国科学院上海有机化学研究所
SIOC
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Content

Welcome to
Shanghai Institute of Organic Chemistry

On behalf of the Shanghai Institute of Organic Chemistry (SIOC), I would like to extend a warm welcome to all participants of the Thieme-SIOC International Symposium on Organic Chemistry. Established in May 1950 as one of the founding institutes of the Chinese Academy of Sciences (CAS), SIOC has continuously advanced the frontiers of organic chemistry and related disciplines. Our State Key Laboratory of Chemical Biology, an evolution of the former State Key Laboratory of Bioorganic and Natural Products Chemistry, now integrates research teams from the Shanghai Institute of Materia Medica (SIMM). This integration combines deep expertise in chemical biology, synthetic chemistry, synthetic biology, structural biology, and medicinal chemistry, creating a unique platform to address the challenges of therapeutic target discovery and validation.

We hope this symposium offers a stimulating and enriching experience, sparking meaningful discussions and fostering new collaborations. Welcome to SIOC, and may your time here be both inspiring and memorable.

Ang Li
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences

Webpage:
http://english.sioc.cas.cn/

Welcome - Willkommen - 欢迎

Dear Colleagues,

Thieme is delighted to be co-organizing this Organic Chemistry Symposium in collaboration with **Shanghai Institute of Organic Chemistry.** We would like to give special thanks to our hosts **Professor Ang Li** and his colleagues for agreeing to co-host this symposium. It is the first time for Thieme Chemistry to have this kind of symposia series in China where we are joined by leading scientists/editors from internationally as well as locally.

The chemical sciences portfolio consists of 11 journals: ***Synthesis, Synlett, SynOpen, Synfacts, Organic Materials, Planta Medica, Pharmacopsychiatry, Drug Research, Pharmaceutical Fronts, Chinese Medicine and Natural Products***, and the newly announced launch of open access journal, ***Sustainability & Circularity Now***. More details can be read on our website. In addition, Thieme also publishes databases such as ***Science of Synthesis, Roempp and Pharmaceutical Substances***. We are a family run publishing house, established in 1886, with headquarters based in Stuttgart, Beijing, New York, Rio de Janeiro, London, and Delhi. Our Editorial colleagues are proud to provide services to our authors, reviewers, readers, and editors from those offices.

We offer one of the fastest times from submission to first decision on manuscripts via our innovative peer review system called ***Select Crowd Review***. This new method of peer review has proven to be fast, efficient, and fair. We would like to encourage postdocs and early career chemists to try this new method of peer review. We are also lucky to have one of the most high-profile networks of organic chemists in the world. At SIOC, we are delighted to have **Professor Ang Li** and **Professor Tiansheng Mei** serve on our editorial boards.

We are pleased to be joining colleagues from China to share our exciting ideas in research with this audience. Plus, we are delighted to have this opportunity to share our experiences of scientific publication, whether as authors or editors, so that we can understand more clearly how our journals can best serve the global scientific community. Our motto at Thieme is to support our community for “Better Health and Better Life”.

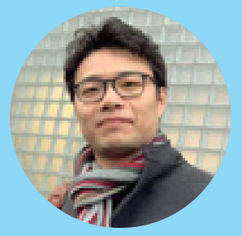
We would like to thank all speakers, organizers, editors, and committee members especially our Editorial Board and Advisory Board members. We hope that all presentations will stimulate exchange of ideas, experiences, and potentially foster future research collaborations.

Welcome to what promises to be an exciting meeting!

Veronika Spinka
Senior Vice President, Thieme Science

Kathleen Too
Senior Vice President, Thieme Chemistry
Managing Director, Thieme China

Stuart Beardsworth
Senior Publisher, Biosciences Journals



Yingxiao Cai
Publisher Acquisitions, Thieme Chemistry

Agenda

Time	Speaker	Title of lecture
09:00 – 09:15	**Prof. Ang Li,** SIOC CAS 李昂 教授 / 上海有机化学研究所	Welcome from the host and inaugural speech
09:15 – 09:30	**Dr. Kathleen Too** Senior Vice President, Thieme Chemistry Managing Director, Thieme China	Thieme Presentation, Introduction of new journals + Group Photo (in the conference room)
09:30 – 10:10	**Prof. Thierry Ollevier** Université Laval, Canada	Design and Applications of Chiral Iron Complexes for Asymmetric Catalysis
10:10 – 10:50	**Prof. Yan Zhang,** Nanjing University 张艳 教授 / 南京大学	Photo-controllable bioorthogonal reactions and biomolecules
10:50 – 11:30	**Prof. You-Cai Hu,** Peking Union Medical College 胡友财 教授 / 北京协和医学院	Glycosylated enzyme-catalyzed tandem [4+2] cycloadditions
11:30 – 13:30	Lunch	
13:30 – 14:10	**Prof. Lu Zhou,** Fudan University 周璐 教授 / 复旦大学	ABPP-CoDEL: A high-throughput screening platform for covalent ligand discovery
14:10 – 14:50	**Prof. Yi-Yun Chen,** SIOC CAS 陈以昀 教授 / 上海有机化学研究所	Biocompatible Photochemistry
14:50 – 15:20	Coffee Break	
15:20 – 16:00	**Prof. Debabrata Maiti,** Indian Institute of Technology Bombay, Indian	Unlocking new chemical space via selective catalysis
16:00 – 16:40	**Prof. Corinna Schindler** University of British Columbia, Canada	Azetidines, Azetines, and Oxetanes: New Cycloadditions of Imines and Carbonyls
16:40 – 17:10	Panel Discussion: What do Editors look for when they assess a paper?	
17:10 – 17:20	**Prof. Ang Li,** SIOC CAS 李昂 教授 / 上海有机化学研究所 **Dr. Kathleen Too** Senior Vice President, Thieme Chemistry Managing Director, Thieme China	Closing Remarks

Symposium President

PROFESSOR

Ang Li

Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences

Associate Editor, Synlett

Lab webpage:
http://angligroup.sioc.ac.cn/

Abstracts and Biographies

PROFESSOR

Thierry Ollevier

Département de Chimie, Université Laval, Canada
Editor-in-Chief, SynOpen

Thierry Ollevier was born in Brussels and obtained his B.Sc. (1991) and Ph.D. (1997) at the Université of Namur (Belgium), and was research associate at the Université catholique de Louvain (Belgium), under I. E. Markó (1997), NATO postdoctorate fellow at Stanford University under B. M. Trost (1998–2000), then postdoctorate fellow at the Université de Montréal under A. B. Charette (2000–2001). After an Assistant Professor appointment (2001) at Université Laval (Québec, Canada), he became Associate (2006) and is currently Full Professor. Current research in his group aims at designing novel catalysts, developing catalytic reactions and applying these methods to chemical synthesis. He is active in the areas of iron catalysis, ligand design, asymmetric catalysis, fluorine chemistry, diazo and diazirine chemistry, flow chemistry, and bismuth chemistry. He has published more than 85 papers and 35 encyclopedia articles and book chapters. He has served as an Associate Editor of RSC Advances from 2015 to 2022 and was admitted as a Fellow of the Royal Society of Chemistry (2016). After 5 years served as Advisory Board member of ***SynOpen***, he has been appointed as Editor-in-Chief of ***SynOpen*** in 2023.

Lab webpage:
http://www2.chm.ulaval.ca/tollevier/

Design and Applications of Chiral Iron Complexes for Asymmetric Catalysis

Thierry Ollevier
Department of Chemistry, Université Laval, Québec, Canada
thierry.ollevier@chm.ulaval.ca

Various iron-derived Lewis acids have been developed as green catalysts in asymmetric synthesis. Chiral iron complexes have been employed in selected asymmetric C–C, C–N, and C–S bond-forming reactions, such as the Mukaiyama aldol, epoxide opening, thia-Michael and Diels-Alder reactions.[1-6] As part of our ongoing interest in ligand design, we report the fine-tuning of alternate designer ligands toward higher chiral inductions. Iron coordination chemistry will be discussed in the context of the enantiocontrol of selected reactions. We developed an efficient chiral C_2-symmetric *2,2′-bipydiol* ligand possessing an adamantyl or a CF_3 group in the α,α′-positions. A highly enantioselective method for the catalytic addition of thiols to α,β-unsaturated oxazolidinones was developed using Fe^{II} salts with the (*S,S*)-2,2′-bipyridine-α,α′-*t*Bu-diol ligand (Bolm's ligand, up to 86% *ee*)[5] and the analogue ligand possessing 3,3′-dimethyl substituents (up to 90% *ee*).[2] The Fe^{III}-catalyzed asymmetric Diels–Alder reaction of various dienes with α,β-unsaturated oxazolidinones was performed using Bolm's ligand (up to 98% *ee*)[3] and the adamantyl-variant (*S,S*)-2,2′-bipyridine-α,α′-1-Ad-diol (up to > 99.5% *ee*).[1] Another new 2,2′-bipydiol ligand possessing CF_3 groups in the α,α′-positions was prepared and used in the asymmetric addition of Et_2Zn to aldehydes (up to 95% *ee*).[4] Overall, the following asymmetric reactions will be presented: Fe^{II}-catalyzed thia-Michael (up to 90% *ee*),[5] Fe^{II}-catalyzed Mukaiyama aldol (up to 98% *ee*),[1,2] Fe^{III}-catalyzed Diels–Alder (up to > 99.5% *ee*),[1,3] and Zn^{II}-mediated Et_2Zn addition to aldehydes (up to 95% *ee*).[4]

Keywords: asymmetric catalysis, chiral ligand, enantioselectivity, iron catalysis

References

1.Lauzon, S.; Schouwey, L.; Ollevier, T. *Org. Lett.* **2022**, *24*, 1116.
2.Lauzon, S.; Caron, L.; Ollevier, T. *Org. Chem. Front.* **2021**, *8*, 2242.
3.Li, M.; Carreras, V.; Jalba, A.; Ollevier, T. *Org. Lett.* **2018**, *20*, 995.
4.(a) Lauzon, S.; Ollevier, T. *Chem. Commun*. **2021**, *57*, 11025; (b) Lauzon, S.; Ollevier, T. *Chem. Sci.* **2022**, *13*, 10985.
5.Lauzon, S.; Keipour, H.; Gandon, V.; Ollevier, T. *Org. Lett.* **2017** *19*, 6324.
6.Bouzid, S.; Marcoux, A.; Ollevier, T. *Chem. Eur. J.* **2024**, *30*, doi: 10.1002/chem.202402449.

PROFESSOR

Yan Zhang

School of Chemistry and Chemical Engineering
Nanjing University

Yan Zhang got her Ph.D in 2002 from Nanjing University, China. She worked as postdoctoral research associate in Hong Kong University of Science and Technology from 2002 to 2004. In 2004-2006, she worked as postdoctoral fellow at the medical school of Stanford University. She joined Nanjing University in the September of 2006 as a professor. Her main research interest is the development of photo-driven bioorthogonal reactions and biological applications of photo-sensitive probes.

Lab webpage:
https://hysz.nju.edu.cn/yanzhang/

Photo-controllable bioorthogonal reactions and biomolecules

Yan Zhang
School of chemistry and chemical engineering, Nanjing University, Nanjing, China
njuzy@nju.edu.cn

Photo-driven bioorthogonal reactions add spatial-temporal resolution to bioorthogonal reactions using photo-irradiation, which may provide photo-controllable molecular tools in chemical biological studies. We have established the visible-light-driven bioorthogonal DVPC reaction of the o-dione (9,10-phenanthrenequinone) with the electron-rich alkene (vinyl ether), which proceeded via the single electron transfer (SET) from the vinyl ether to the photo-excited state of o-dione as the first bioorthogonal bond-forming step[1]. The presence of water in biological systems was used as “polar solvent cages” of the excited state to block side reactions and realize bioorthogonality. Spatial-temporal labeling of antibodies on live cells was achieved using DVPC. DVPC was also orthogonal to the strain-promoted azide alkyne click reaction (SPAAC), which enabled orthogonal labeling of two proteins in one batch. Further exploration on the cycloaddition reactions between o-diones and other electron-rich C=C bonds led to the discovery of the bioorthgonal DFC reaction[2], which was the first anionic cycloaddend-promoted bioorthogonal cycloaddition reaction. With the water-mediated formation of the highly electron-rich anionic cycloaddend from furan-2(3H)-one derivatives, which is stabilized in water with high polarity, the DFC reaction with ground state o-diones proceeds rapidly in aqueous solution and in live cells. The combined utilization of this reaction together with the two other widely used bioorthogonal reactions SPAAC and IEDDA allows for mutually orthogonal labelling of three types of proteins or three groups of living cells in one batch without cross-competition. Using bioorthogonal reactions, we were able to build various bio-active molecules to visualize or regulate biological systems with spatial and temporal resolution.[3-5]

Keywords: bioorthogonal reaction, photo-driven, DVPC, DFC

References

[1] Li, J.; Kong, H.; Huang, L.; Cheng, B.; Qin, K.; Zheng M.; Yan, Z.; Zhang, Y. *J. Am. Chem. Soc.* **2018**, *140*, 14542-14546.
[2] Xi, Z.; Kong, H.; Chen, Y.; Deng, J.; Xu,W.; Liang, Y.; Zhang, Y. *Angew. Chem. Int. Ed.*, **2022**, e202200239.
[3] Wang, Y.; Weng, J.; Lin, J.; Ye, D.; Zhang, Y. *J. Am. Chem. Soc.* **2020**, *142*, 2787-2794.
[4] Wang,Y.; Bai, H.; Miao, Y.; Weng, J.; Huang, Z.; Fu, J.; Zhang, Y.; Lin, J.; Ye, D. *Angew. Chem. Int. Ed.* **2022**, e202200369.
[5] Zhu, C., Wang, W., Wang, Y., Zhang, Y., Li, J. *Angew. Chem. Int. Ed.* **2023**, e202300694.

PROFESSOR

You-Cai Hu

Peking Union Medical College
Chinese Academy of Medical Sciences

Youcai Hu received his Ph.D. degree in 2008 from Peking Union Medical College (PUMC), where he studied natural medicinal chemistry with Prof. Shishan Yu. After postdoctoral training on marine natural products (2010-2013, with Prof. John B. MacMillan), and natural product biosynthesis (2013-2014, with Prof. Yi Tang), he returned to Institute of Materia Medica, PUMC in end of 2014. His research interests focus on genome mining guided discovery and biosynthesis of natural products as well as drug discovery.

Lab webpage:
https://pumc.teacher.360eol.com/teacherBasic/preview?teacherId=3287

Glycosylated enzyme-catalyzed tandem [4+2] cycloadditions

Youcai Hu
State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, China.
huyoucai@imm.ac.cn

Tandem Diels-Alder reactions are frequently employed in the synthesis of complex organic compounds with polycyclic ring systems. Bistropolone-sesquiterpenes, such as eupenifeldin and pycnidione, possess a complex pentacyclic ring system. These optically active compounds were isolated with low yield from fungi and have been reported by pharmaceutical companies Bristol–Myers Squibb and Merck Sharp & Dohme to exhibit nanomolar antitumor activity. The total chemical synthesis of these compounds remains challenging, and none have been synthesized. We present the heterologous biosynthesis of these compounds using a key tandem cycloaddition enzyme. Unlike most single-cycloaddition catalyzing enzymes (e.g., DAases), enzymes capable of facilitating multiple Diels-Alder reactions are rare. Herein, we demonstrate that two glycosylated enzymes, EupfF and PycR1, which depend on calcium ions for activity, independently catalyze sequential intermolecular Diels-Alder reactions during the biosynthesis of eupenifeldin and pycnidione. [1-2]

We also elucidate the origins of catalysis and stereoselectivity within these DAases through analysis of enzyme co-crystal structures, together with computational and mutational studies. These enzymes are secreted as glycoproteins with diverse N-glycans. The N-glycan at N211 in PycR1 significantly enhances the affinity to the calcium ion, thereby regulating the active cavity specifically for substrate interaction and accelerating the tandem [4 + 2] cycloaddition reaction. The synergistic effect of calcium ions and N-glycans on the catalytic center of enzymes involved in secondary metabolism, particularly for complex tandem reactions, expands our understanding of protein evolution and advances artificial design strategies for biocatalysts.[3]

Keywords: Biosynthesis, tandem [4 + 2] cycloadditions, protein glycosylation, Diels-Alderase, calcium ions

References

[1]. Liu J. W., Lu J.Y., Zhang C., X., Zhou Q.Y., Jamieson C.S., Shang C.S., Houk N.C.*, Zhou J.H.*, Hu Y.C.*, *Nat. Chem.*, **2023**, *15 (8)*, 1083-1090.
[2]. Che Q. B., Gao J., Jamieson C.S., Liu J.W., Ohashi M., Bai J., Yan D.J., Liu B.Y., Che Y.S., Wang Y.N., Houk N.C.*, Hu Y.C.*, *J. Am. Chem. Soc.*, **2019**, *141 (36)*, 14052-14056.
[3]. Liu J. W., Hu Y.C.*, *Curr. Opin. Chem. Biol.*, **2024**, *81*, 102504.

PROFESSOR

Lu Zhou

School of Pharmacy
Fudan University

Dr. Lu Zhou received his BS degree in Chemistry at Peking University and obtained Ph.D. in Physical Chemistry at Peking University in 2006. He received his postdoctoral training in Chemical Biology in the Chemistry Department at the University of Chicago. In 2012, he was recruited to Fudan University, where he was appointed as an assistant professor and promoted to full professor in 2020. Current research in his lab focuses on the discovery of small-molecule modulators against enzymes involved in glucose and lipid metabolism. His research provides “prove of concept” of metabolic enzymes as novel therapeutic targets. He has authored over 80 scientific publications and 10 patents.

Lab webpage:
https://spfdu.fudan.edu.cn/53/4e/c44887a676686/page.htm

ABPP-CoDEL: A high-throughput screening platform for covalent ligand discovery

Lu Zhou
Department of Medicinal Chemistry, School of Pharmacy, Fudan University, Shanghai, P.R. China
zhoulu@fudan.edu.cn

Covalent drugs have proven to be successful therapies for various diseases over the past century. Owing to safety concerns, they are rarely considered as the first choice when initiating a target-directed drug discovery project. More recently, tools that facilitate high-throughput screening of covalent drugs have emerged. Incorporating an electrophile warhead into DNA-encoded compounds has recently permitted the discovery of covalent ligands that selectively react with a particular cysteine residue. However, non-cysteine residues remain underexplored as modification sites for covalent DELs. Herein, we report the design and utility of tyrosine-targeting DELs. Proteome-wide reactivity analysis of tyrosine-reactive sulfonyl fluoride (SF) covalent probes suggested three enzymes as models for tyrosine-targetable proteins. Enrichment with SF-functionalized DELs led to the identification of a series of tyrosine-targeting covalent inhibitors of these model enzymes. In-depth mechanistic investigation revealed their novel modes of action and reactive ligand-accessible hotspots on the enzymes. Our strategy of combining activity-based proteome profiling and covalent DEL enrichment (ABPP-CoDEL) has generated selective covalent binders against a variety of target proteins, illustrating the potential use of this methodology in further covalent drug discovery.

Keywords: covalent drug, ABPP, DNA encoded library

References

[1] Jiang L, Liu S, Jia X, Gong Q, Wen X, Lu W, Yang J, Wu X, Wang X, Suo Y, Li Y, Uesugi M, Qu ZB, Tan M, Lu X, Zhou L. *J Am Chem Soc.* **2023**,*145(46)*:25283-25292.

PROFESSOR

Yi-Yun Chen

The Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences

Dr. Yiyun Chen is a Professor at the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, and a member of China's State Key Laboratory of Chemical Biology. Having earned his bachelor's degree in chemistry from Peking University in 2002, Chen went on to obtain his Ph.D. in organic chemistry from Princeton University in 2007. His academic journey continued with postdoctoral research in chemical biology at Harvard University and the Howard Hughes Medical Institute. In 2011, Chen joined the Shanghai Institute of Organic Chemistry as a Principal Investigator, focusing his research on biocompatible photochemistry, including organic photochemistry and photochemical biology. Chen has made significant contributions to the field of photochemistry, pioneering the development of cyclic iodine(III) reagents for photocatalytic reactions, unraveling the photocatalytic reactivity of alkoxyl radicals, and more recently, exploring the photochemical rearrangements of organoboronates. His overarching research goal is to create versatile photochemical reactions that are compatible with biological systems, with the ultimate aim of developing innovative photo-diagnostic and photo-therapeutic applications.

Lab webpage:
Group website: http://yiyunchen.sioc.ac.cn
Research group Twitter: @bio_photochem

Biocompatible Photochemistry

Yiyun Chen
Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China.
yiyunchen@sioc.ac.cn

Organic photochemistry offers unique pathways for challenging chemical transformations with high-energy barriers. However, limitations like short-lived excited states and intricate reaction mechanisms hinder their synthetic applications. We present our recent advances in overcoming these hurdles through the study of photochemistry in organic boron, iodine, and oxygen compounds.

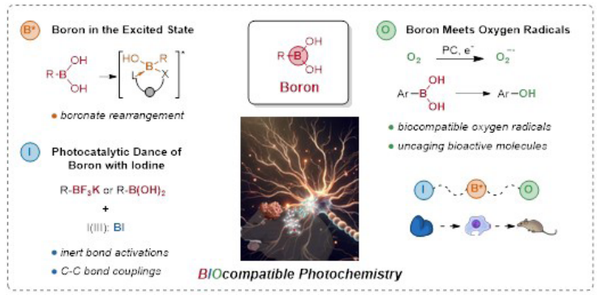
Our work encompasses three key areas:

1. Photorearrangement of Organoboronates: We discovered a novel photorearrangement that overcomes limitations of organoboronate migration, enabling new strategies for high-energy-barrier transformations.[1]

2. Cyclic Hypervalent Iodine(III) Reagents: We developed novel cyclic hypervalent iodine(III) reagents and elucidated unique reactivity at the α-position of alkoxy radicals, expanding the potential of their photochemical reactions.[2]

3. Bioorthogonal Photocatalysis: We established bioorthogonal photocatalytic technology for light-mediated modulation and labeling of biomolecules within living cells and mice, opening doors for biodiagnostic and biomedical applications.[3]

This presentation will explore these findings and their broader implications for organic synthesis, photochemistry, and chemical biology. We will also discuss future directions in unraveling key scientific questions in this exciting field.



Keywords: boron, hypervalent iodine, oxygen radical, photochemistry, biocompatible reaction

References

4.(a) Xie, S.; Chen, Y.* *et al. J. Am. Chem. Soc.* **2019**, 141, 11, 16237. (b) Hao, K.[1]; Li, D.[1]; Lan, Y.*; Chen, Y.* *et al. Angew. Chem. Int. Ed.* **2024**, 63, e202316481.

5.(a) Jia, K., Chen, Y.*, In *PATAI'S Chemistry of Functional Groups*, Marek, I., Olofsson, B., Rappoport, Z., eds. **2018**, 1–42. (b) Huang, H.; Chen, Y.* *et al. J. Am. Chem. Soc.* **2014**, 136, 2280. (c) Huang, H.; Chen, Y.* *et al. Angew. Chem. Int. Ed.* **2015**, 54, 1881. (d) Huang, H.1; Zhang, G.1; Chen, Y.* *et al. Angew. Chem. Int. Ed.* **2015**, 54, 7872. (e) Jia, K.; Chen, Y.* *et al. J. Am. Chem. Soc.* **2016**, 138, 1514. (f) Jia, K.; Chen, Y.* *et al. Angew. Chem. Int. Ed.* **2017**, 56, 2478. (g) Dong, X.1, Shao, Y.1, Chen, Y.* *et al. Angew. Chem. Int. Ed.*, **2024**, e202410297.

6. (a) Zhang, J., Liu, D., Chen, Y.*, *Oxygen-centered radicals, In Science of Synthesis,* **2021**, Vol. 1, 323. (b) Zhang, J.; Chen, Y.* *et al. Angew. Chem., Int. Ed.* **2016**, 55, 1872. (c) Zhang, J.; Li, Y.; Xu, R.; Chen, Y.* *Angew. Chem., Int. Ed.* **2017**, 56, 12619. (d) Zhang, J.; Lan, Y.*; Chen, Y.* *et al. iScience.* **2020**, 23, 100755. (e) Liu, D.; Lan, Y.*; Chen, Y.* *et al. Angew. Chem., Int. Ed.* **2022**, e202213686. (f) Wang, H.; Xu, T.*, Chen, Y.* *et al. Angew. Chem., Int. Ed.* **2019**, 58, 561. (g) Zeng, K.1; Jiao, Z.1; Li, W*, Xu, T*, Chen, Y* *et al. ACS Cent. Sci.* **2024**, 10, 1, 163.

PROFESSOR

Debabrata Maiti

Department of Chemistry, Indian Institute of Technology Bombay
Editor-in-Chief, Synlett

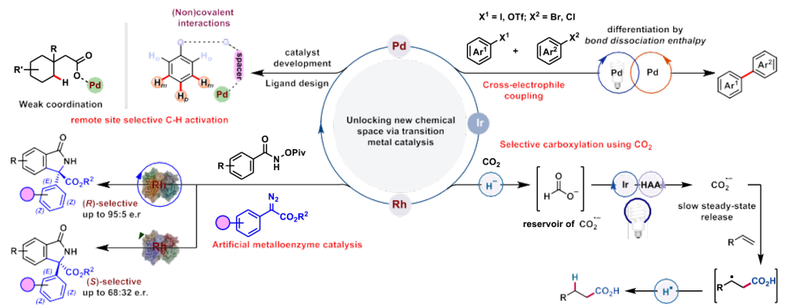
Prof. Debabrata Maiti received his PhD from Johns Hopkins University in 2008 under the supervision of Prof. Kenneth D. Karlin. After postdoctoral studies at MIT with Prof. Stephen L. Buchwald, he joined the Department of Chemistry at IIT Bombay in 2011. His research interests are focused on the development of new and sustainable synthetic and catalytic methodologies. Currently he is *Editor- in-Chief, Synlett*.

Lab webpage:
https://www.dmaiti.com/

Unlocking new chemical space via selective catalysis

Debabrata Maiti
Department of Chemistry, Indian Institute of Technology Bombay
dmaiti@iitb.ac.in

The limitations of cross-coupling such as the availability of prefunctionalized coupling partners, instability, and synthesis expense remain, posing significant barriers to unlocking new chemical space for molecular complexity. To solve these underlying problems of cross-coupling we are mainly focused on the development of techniques for direct C–H functionalization and cross- electrophile coupling. Selectively targeting a remote C–H bond in a molecule remains more challenging due to the inaccessibility of these sites in formation of energetically favorable organometallic pre-transition states. We believe that the direct release of the reactive metal catalyst in close proximity to the targeted remote C–H bond could solve this problem. We devised covalently attached template-directed methods that require precise spatial positioning of the directing group in order to selectively activate remote C–H bonds. We recently demonstrated that various non-covalent interactions are also successful in recognizing the perfect orientation of catalyst and the substrate to achieve selective C–H bond activation. In this vein, we have developed a method for the activation of methylene C–H bond in presence of methyl C–H bonds to form unsaturated bicyclic lactones utilizing the weak coordinating nature carboxylic acid towards palladium. Cross-electrophile coupling (XEC) approach would be a powerful tool for the construction of (hetero)biaryl moiety because of the widespread availability and stability of (hetero)aryl electrophiles. We have demonstrated a ligand controlled visible light driven monometallic cross-electrophile coupling platform for the synthesis of unsymmetrical (hetero)biaryls directly from (hetero)aryl halides and pseudohalides. In addition, our lab is pursuing the development of a paradigm in which small molecules such CO_2, SO_2 *etc*. can be converted into a wide range of chemicals and materials using renewable visible light photocatalysis.



References

1. Dutta, U.; Maiti, S.; Bhattacharya, T.; Maiti, D. Science, 2021, 372, 701.
2. Goswami, N.; Sinha, S. K.; Mondal, P.; Adhya, S.; Datta, A.; Maiti, D. Chem, 2023, 9, 989.
3. Saha, A.; Guin, S.; Ali, W.; Bhattacharya, T.; Sasmal, S.; Goswami, N.; Prakash, G.; Sinha, S. K.; Chandrashekar, H. B.; Panda, S.; Anjana, S. S.; Maiti, D. J. Am. Chem. Soc. 2022, 144, 1929.
4. Das, J.; Ali, W.; Ghosh, A.; Pal, T.; Mandal, A.; Teja, C.; Dutta, S.; Pothikumar, R.; Ge, H.; Zhang, X.; Maiti, D. Nat. Chem. 2023, 15, 1626.
5. Maiti, S.; Ghosh, P.; Raja, D. K.; Ghosh, S.; Chatterjee, S.; Sankar, V.; Roy, S.; Lahiri, G. K.; Maiti, D. Nat. Catal. 2024
6. Mukherjee, P.; Sairaman, A.; Deka, H. J.; Jain, S.; Mishra, S. K.; Roy, S.; Bhaumik, P.; Maiti, D. Nat. Synth. 2024

PROFESSOR

Corinna Schindler

Department of Chemistry, University of British Columbia, Canada
Associate Editor, Synthesis

Corinna was born and raised in Schwaebisch Hall, Germany. As an undergraduate at the Technical University of Munich, she worked in the area of organometallic chemistry. Upon completion of her Diploma Thesis at the Scripps Research Institute in La Jolla in the laboratory of K.C. Nicolaou, she joined the research group of Erick M. Carreira at the ETH Zurich in Switzerland for her graduate studies. During her time in the Carreira group Corinna worked on developing novel synthetic methodologies as well as successful synthetic strategies to access Banyaside A and Microcin SF608. For her postdoctoral studies, Corinna joined the laboratory of Eric N. Jacobsen at Harvard University as a Feodor Lynen Postdoctoral Fellow to work in the field of asymmetric catalysis.

Lab webpage:
https://www.schindlerresearchgroup.com/

Azetidines, Azetines, and Oxetanes: New Cycloadditions of Imines and Carbonyls

Corinna S. Schindler
University of British Columbia, 2036 Main Mall, Vancouver, BC V6T 1Z2
yhl198151@cqu.edu.cn

Four-membered nitrogen heterocycles such as azetidines possess unique properties that make them desirable for drug discovery and synthesis applications. However, synthesis of these compounds is challenging, limiting their applicability. While oxetanes and cyclobutanes are commonly synthesized by highly atom-economical light-mediated [2+2] reactions, this powerful methodology remains limited for the synthesis of azetidines via the aza Paternò-Büchi reaction. Herein we report the development of visible-light mediated intermolecular aza Paternò-Buchi reactions,1-4 harnessing the triplet state of unique cyclic oximes, specifically 2-isoxazoline-3-carboxylates, as imine equivalents for the synthesis of unique azetidine and azetine products. Following energy transfer from an iridium photocatalyst, these cyclic oximes initiate [2+2] reactions with unactivated alkenes and alkynes, allowing access to a broad range of azetidines and azetines with excellent yield. This method is mild, operationally simple, and broadly applicable. Importantly, these products can be easily converted to free monocyclic azetidines, offering a new approach to these desirable targets.

References

1. Wearing, E.R.; Blackmun, D.E.; Becker, M.R.; Schindler, C.S. *J. Am. Chem. Soc.* **2021**, *143*, 16235-16242.
2. Becker, M.R.; Wearing, E.R.; Schindler, *C.S. Nat. Chem.* **2020**, *12*, 898–905.
3. Becker, M.R.; Richardson, A.D.; Schindler, *C.S. Nat. Commun.* **2019**, DOI: 10.1038/s41467-019-13072-x.
4. Wearing, E.R.; Yeh, Y.-C.; Terrones, G.G.; Parikh, S.G.; Kevlishvili, I.; Kulik, H.J.; Schindler, *C.S. Science* **2024**, *384*, 1468-1476.

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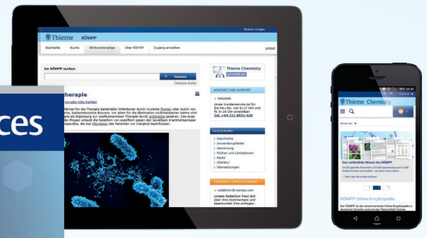

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