



The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Dr. John C.K. Chu
Colorado State University
U.S.A.

Title: Synthesis of Nitrogen-Containing Molecules by Zinc-Catalyzed [4+2] Cycloaddition and Photoredox-Catalyzed C-H Functionalization

Date: March 1, 2017 (Wednesday)

Time: 2:00 p.m.

Venue: Room G04, Y.C. Liang Hall

< Abstract >

The overwhelming presence of nitrogen atoms in pharmaceuticals highlights the pressing need for organic chemists to streamline and accelerate the synthesis of nitrogen-containing molecules. This seminar will discuss two projects in my Ph.D studies that aimed to address the limitations of amine synthesis. The first project is on zinc-catalyzed enantioselective [4+2] cycloaddition of 1-azadienes and nitro-alkenes to access piperidine derivatives.¹ This reaction represents a rare example of [4+2] cycloadditions of two electron-deficient dienes and alkenes. The second project is on a photoredox-catalyzed C-C bond formation reaction at unactivated sp³ C-H bonds using nitrogen as a directing group.² In this approach, pre-functionalization of a N-H bond is not required for the generation of the nitrogen radical, the intermediate responsible for the cleavage of the inert C-H bond through hydrogen atom transfer. The scope and mechanistic aspects of the two reactions will be discussed.

1. *J. Am. Chem. Soc.* **2015**, *137*, 4445-4452
2. *Nature* **2016**, *539*, 272-275.

Biography

John obtained his BSc in Chemistry with a first-class honors at the University of Hong Kong. As an undergraduate researcher, he worked with Profs Pauline Chiu (HKU), Michael Chong (Waterloo, Canada) and Steven Ley (Cambridge, England). As a Croucher scholar, he pursued PhD studies with Prof. Tomislav Rovis at Colorado State University. With a Marie-Curie fellowship, he will begin work as a postdoctoral researcher with Prof. Matthew Gaunt at the University of Cambridge in March 2017.



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Speaker: Prof. Wei Han
School of Chemical Biology and Biotechnology
Peking University Shenzhen Graduate School

Title: In silico Insights into Protein Aggregation

<< *Abstract* >>

Uncontrollable self-assembly of misfolded or natively unfolded proteins is a central molecular event behind numerous neurodegenerative diseases such as Alzheimer's and Parkinson's diseases as well as type II diabetes. Understanding these processes with atomic details is invaluable for disease treatment. Molecular simulations have served as an indispensable tool for providing details of protein conformational change but their application in this regard is hampered by computational challenge in exploring extremely complicated free energy landscape of the protein self-assembly and associated kinetics. In this talk, I will present our computational effort in understanding the mechanism of protein self-assembly. A hybrid-resolution model is devised to overcome the computational challenge. Furthermore, a method based on Markov state model is also developed and applied to systematically examine structural transitions during the self-assembly. These approaches, when combined, permit us to derive detailed kinetic pictures of two key stages of the protein self-assembly, namely nucleation and elongation, providing numerous insights. Finally, I will also discuss our recent computational attempt to employ molecular simulations to assist in seeking means of retarding the process of protein self-assembly. Together, our studies reveal potential value of molecular simulations for tackling the problem of the protein aggregation.

Date: March 21, 2017 (Tuesday)
Time: 2:30 p.m.
Venue: Room G35, Lady Shaw Building



ALL ARE WELCOME

Contact Person:
Prof. Steve Y.L. Tse



The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Prof. Heikki Tenhu
Department of Chemistry
University of Helsinki
Finland

Title: Polymers and particles from N-vinylcaprolactam

Date: March 22, 2017 (Wednesday)

Time: 2:30 p.m.

Venue: Room C1
Lady Shaw Building



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Contact Person:
Prof. Chi Wu



The Chinese University of Hong Kong

Department of Chemistry

Research Seminar Series

Speaker: Prof. Heikki Tenhu
Department of Chemistry
University of Helsinki
Finland

Title: Polymeric hybrid nanomaterials

Date: March 24, 2017 (Friday)

Time: 4:30 p.m.

Venue: L1
Science Centre



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Contact Person:
Prof. Chi Wu



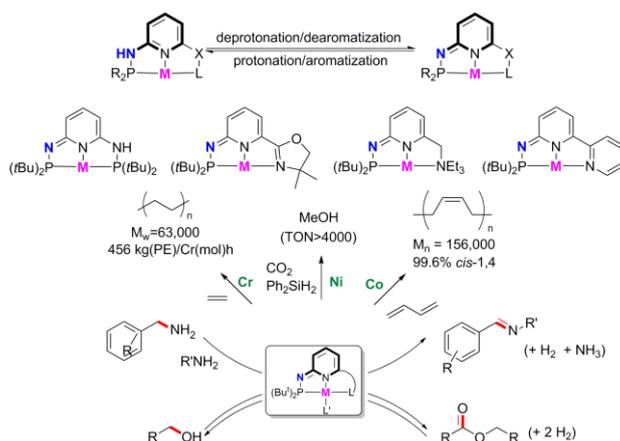
The Chinese University of Hong Kong
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Research Seminar Series

Speaker: Prof. Kuo-Wei Huang
KAUST Catalysis Center and Division of Physical Science and Engineering
King Abdullah University of Science and Technology, Saudi Arabia

Title: A Novel Class of PN₃-Pincer Complexes: Cooperative Catalysis and Beyond

<< Abstract >>

Pincer transition metal complexes have versatile reactivities to catalyze many organic transformations and to activate strong chemical bonds. In particular, complexes with ligand derived from tridentate pyridine-based framework exhibit interesting reactivities. We have designed and prepared a series of transition metal catalysts based on a novel class of pincer-type PN₃ ligands which are capable of interacting with the substrates during the reaction. Rich reactivities have been observed with their catalytic activities being explored recently. In very recent work, we have witnessed that the seemingly small change by replacing the CH₂ spacer in the pyridine-based pincer complex with an NH group has dramatically influenced the thermodynamic and kinetic properties, and in some cases the catalytic behaviors of the corresponding metal complexes. It is conceivable that this new class of transition metal pincer complexes will offer exciting opportunities for the development of novel catalytic applications in the petrochemical and energy sectors.



References

- [1] Li, H.; Zheng, B.; Huang, K.-W. *Coord. Chem. Rev.* **2015**, 293-294, 116-138.
- [2] Zeng, G.; Chen, T.; He, L.-P.; Pinnau, I.; Lai, Z.-P.; Huang, K.-W. *Chem. Eur. J.* **2012**, 18, 1594.
- [3] Qu, S.; Dang, Y.; Song, C.; Wen, M.; Huang, K.-W.; Wang, Z.-X. *J. Am. Chem. Soc.* **2014**, 136, 4974.
- [4] Chen, T.; Li, H.; Qu, S.; Zheng, B.; Lai, Z.-P.; Wang, Z.-X.; Huang, K.-W. *Organometallics* **2014**, 33, 4152.

Date: March 29, 2017 (Wednesday)

Time: 2:30 p.m.

Venue: Room 158, Science Centre



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Contact Person:
Prof. Y.Y. Yeung



*The Chinese University of Hong Kong
Research Seminar Series*

Jointly Organized by
Department of Chemistry and School of Life Sciences

- Speaker:** Prof. Hue Sun Chan
Departments of Biochemistry and Molecular Genetics
University of Toronto
- Title:** Biophysics of Protein Evolutionary Switches and Phase Separation in Membraneless Organelles
- Date:** March 29, 2017 (Wednesday)
- Time:** 4:30 p.m.
- Venue:** L5, Science Centre

< Abstract >

How might new protein folds evolve without detrimental effects on the biological function being performed by the original structural fold?

Recent studies by many laboratories indicate that selection of latent "promiscuous" traits can be an efficient route to new function, and that the adaptive conflict between the old and new folds can be resolved by gene duplication and intrinsic kinetic effects of sequence-space topology. Intense research in the past one and a half decade has also demonstrated that not all proteins function as folded structures.

Intrinsically disordered proteins (IDPs) or protein regions perform critical physiological functions, especially for the regulation of cellular processes in higher organisms. Remarkably, some IDPs function not only as individual molecules, but also collectively by undergoing reversible liquid-liquid phase separation in the living cell.

The resulting high-IDP phase forms a major component of membraneless organelles such as P granules and nucleolus that, by creating their own IDP-rich compartments, stimulate critical biological functions.

To gain physical insight into these newly discovered and fascinating phenomena, I will discuss recent effort in using computational models and analytical theory to elucidate how new protein folds might have arisen in evolution and how biologically functional phase separation of IDPs is governed by their genetically coded amino acid sequences.

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Contact Person:
Prof. Jiang Xia



The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Prof. Young-Tae Chang
 National University of Singapore

Title: Fluorescent Sensor Development for Almost Everything

Date: March 31, 2017 (Friday)

Time: 4:30 p.m.

Venue: L1, Science Centre

<< Abstract >>

Conventional sensor development requires defining the target and design of sensor, which is so-called hypothesis driven approach. While powerful, this approach cannot be applied to unknown target or difficult to be applied to complex of analytes. To overcome the limitation, we have devised a Diversity Oriented Fluorescence Library Approach (DOFLA) where a combinatorial synthesis of fluorescent dye is combined with unbiased screening to accelerate the sensor development. More than 10,000 synthetic organic dyes were constructed as a tool box, and numerous analytes have been tested, yielding systematic platform for sensor development for almost everything. Not only physical analytes, phantom target such as “temperature” is also pursued with biological application. Complex or unknown target problem with biological systems were also challenged, and various cell type selective probes for live bioimaging were developed. The sensors and probes developed in this study will be freely available for the chemical and biological community for common usage.

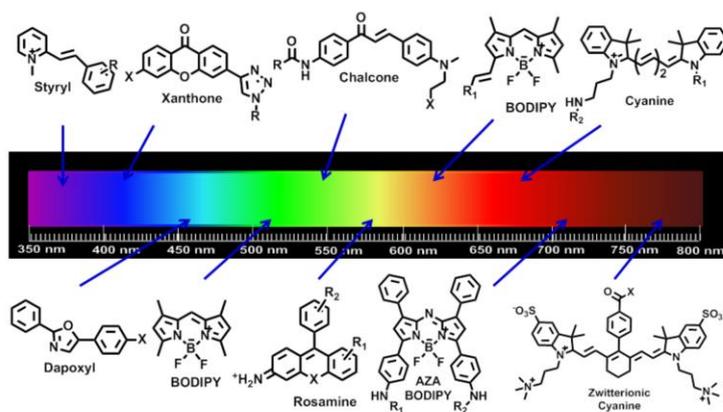


Figure 1. Structure of Diversity Oriented Fluorescence Library

Young-Tae Chang was born in Busan, Korea, in 1968. He studied chemistry in Pohang University of Science and Technology (POSTECH, Korea) and received his B.S. in 1991. After one and half years of army service in Korea, he started his graduate study at POSTECH and received a Ph.D. in 1997 under the supervision of Prof. Sung-Keek Chung, working on the divergent synthesis of all possible regioisomers of myo-inositol phosphates. He did his postdoctoral work with Prof. Peter Schultz at UC Berkeley and The Scripps Research Institute. In 2000, he was appointed assistant professor at New York University and promoted to associated professor in 2005. He received the NSF Career award in 2005 and his research interests have been chemical genetics, molecular evolution, and artificial tongues. In September, 2007, he moved to National University of Singapore and Singapore Bioimaging Consortium. He is a full professor of Chemistry and leader of Medicinal Chemistry Program of NUS, and Lab Head of Bioimaging Probe Development at SBIC, Biopolis. He published more than 300 scientific papers / 3 books and filed 50 patents so far.

