

*The Chinese University of Hong Kong*

*Department of Chemistry*

*Research Seminar Series*

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**Speaker:** Prof. Robert Grubbs  
Nobel Laureate in Chemistry 2005  
Victor and Elizabeth Atkins Professor of Chemistry  
Division of Chemistry and Chemical Engineering  
California Institute of Technology  
U.S.A.

**Title:** Design of Selective Metathesis Catalysis

**Date:** October 6, 2016 (Thursday)

**Time:** 12:30 p.m.

**Venue:** LT1  
Lee Shau Kee Building



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Contact Person:  
Prof. H.K. Lee



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

**Speaker:** Prof. Jiahai Zhou  
State Key Laboratory of Bio-organic  
Chemistry and Natural Products  
Shanghai Institute of Organic Chemistry  
Chinese Academy of Sciences

**Title:** Structural enzymology in biocatalysis and  
biosynthesis

**Date:** October 6, 2016 (Thursday)

**Time:** 3:30 p.m.

**Venue:** L2  
Science Centre



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Contact Person:  
Prof. Jiang Xia



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

**Speaker:** Prof. Richard M.W. Wong  
 Head, Department of Chemistry  
 National University of Singapore

**Title:** Catalytic Activity and Stereoselectivity of Organocatalysts: Interplay of Non-covalent Interactions

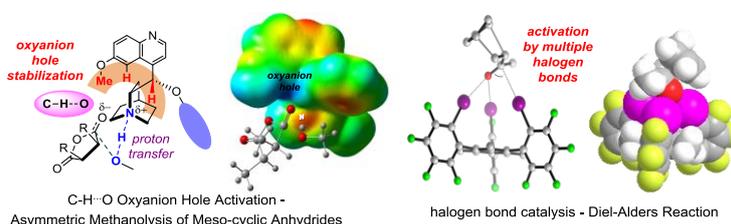
**Date:** October 14, 2016 (Friday)

**Time:** 4:30 p.m.

**Venue:** L1, Science Centre

< Abstract >

This presentation highlights the role of non-covalent interactions in understanding catalytic mechanism and origin of stereoselectivity in organocatalysis. Non-covalent interactions, such as hydrogen bond, are the key to understand mode of activation in organocatalytic systems. Weaker non-covalent forces, such as C-H $\cdots$ O interaction,  $\pi\cdots\pi$  stacking, etc, could interact cooperatively to influence stereoselectivity of asymmetric reactions. For instance, several C-H's (termed "C-H oxyanion hole") could stabilize a transition state with developing oxyanion, via multiple C-H $\cdots$ O interactions in a cooperative manner. The balance of attractive non-covalent forces together with destabilizing repulsion interactions hold the key to discern differential stabilization (or destabilization) of stereoisomeric transition states, which aid to unravel the origin of stereocontrol in organocatalytic reactions. Computational chemistry offers a vital and complementary tool to gain insight into reaction mechanism, mode of activation and origin of stereoselectivity in organocatalysis. Here, several examples of our computational studies on organocatalytic reactions are given. Each of these examples reveals different type of unconventional non-covalent interaction in transition state.<sup>1-4</sup> In each case, the DFT calculations shed light on the underlying mechanism and mode of asymmetric induction and readily explain the observed enantioselectivity.



#### References

1. Yang, H.; Wong, M. W. *J. Am. Chem. Soc.* **2013**, *135*, 5808.
2. Xue, H.; Jiang, D.; Jiang, H.; Kee, C. W.; Hirao, H.; Nishimura, T.; Wong, M. W.; Tan, C.-H. *J. Org. Chem.* **2015**, *80*, 5745-5752.
3. Kee, C. W.; Wong, M. W. *J. Org. Chem.* **2016**, *81*, 7475.
4. Wong, M. W. Yang, H.; Kee, C. W. *Acc. Chem. Res.* accepted.



#### Richard Ming Wah Wong

Australian National University (Ph.D., 1988, Prof. Leo Radom)  
 IBM Kingston (Postdoc, 1989, Prof. Enrico Clementi)  
 Yale University (Postdoc, 1990-1991, Prof. Kenneth B. Wiberg)  
 University of Queensland (Australian Research Fellow, 1992-1996)  
 National University of Singapore (Senior Lecturer, Associate & Full Professor, 1997-present)  
 Field of research: computational quantum chemistry, physical organic chemistry, catalysis  
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*The Chinese University of Hong Kong*  
*Department of Chemistry*  
*Research Seminar Series*

- Speaker:** Prof. Guigen Li  
 Department of Chemistry & Biochemistry, Texas Tech University  
 Institute of Chemistry & BioMedical Sciences, Nanjing University
- Title:** Greener Catalytic and Synthetic Chemistry and Technology
- Date:** October 21, 2016 (Friday)
- Time:** 4:30 p.m.
- Venue:** L1, Science Centre

<< Abstract >>

Organic synthesis and related pharmaceutical and material sciences have been labeled by environmental pollution for a long time, which is due to the use of toxic additives/promoters, the generation of by-products and wastes, and particularly, the use of substantial amounts of silica gels and solvents for chromatography purification. For example, a 15 people's synthetic group, the annual need of silica gels and solvents is about 500 kg and 1000 L, respectively, that are all discarded after each use. In the meanwhile, transition metal catalysis and synthesis has been predominantly pursued in several decades. The search for less toxic and more efficient catalytic reactions, especially, extremely challenging ones, has been actively conducted in organic and organometallic chemistry.

This talk will be focused on: (1) Group-Assisted Purification chemistry (GAP chemistry) to avoid the traditional way of purification, such as column chromatography and recrystallization; (2) Group-Assisted Synthesis chemistry (GASyn chemistry) to enhance reaction efficiency and selectivity by designing powerful auxiliaries attached onto substrates, and related auto synthesizers based on the above GAP and GASyn chemistry; (3) Transient ligand/metal-catalyzed site-selective C–H bond activation on unactivated  $sp^3$  carbons with the assistance of a bidentate directing group, and the direct arylation of aliphatic aldehydes via the metal-catalyzed  $sp^3$  C–H bond functionalization by using 3-aminopropanoic acid as a transient directing group.

**Keywords** GAP chemistry; GASyn chemistry; transition metal catalysis; C-H functionalization.

**References**

1. An, G.; Seifert, C.; Li, G. *Org. Biomol. Chem.* **2015**, *13*, 1600.
2. Li, Q.; Li, Y.; Hu, W.; Hu, R.; Li, G.; Lu, H. *Chem. Eur. J.*, **2016**, *22*, 12286.
3. Wu, X.; Yang, K.; Zhao, Y.; Fan, W.; Sun, H.; Li, G.; Ge, H. *Nature Commun.* **2015**, *6*, 6462.
4. Qiu, J.; Jiang, B.; Zhu, Y.; Hao, W.; Wang, D.; Sun, P.; Wei, P.; Tu, S.; Li, G. *J. Am. Chem. Soc.*, **2015**, *137*: 8928.
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*The Chinese University of Hong Kong*  
*Department of Chemistry*  
*Research Seminar Series*

**Speaker:** Dr. Dieter Klaus Lilge  
Former Head, Polymer Physics and  
Characterization (PP&C) Laboratory  
Lyondellbasell, Industriepark Höchst  
Germany

**Title:** Polyethylene – a versatile Polymer -  
Characterisation and Applications

**Date:** October 21, 2016 (Friday)

**Time:** 2:30 p.m.

**Venue:** LT3  
Lady Shaw Building





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

**Speaker:** Prof. Frédéric Lamaty  
Institut des Biomolécules Max Mousseron  
CNRS-Universités de Montpellier, France

**Title:** Mechanochemistry and its applications: from organic and peptide synthesis to organometallics and catalysis

<< Abstract >>

**Keywords:** solvent-free, ball-milling, biomolecules, peptides, organometallics, catalysis

A major concern for the development of a sustainable chemical synthesis is the use of organic solvents. These solvents are very often toxic and volatile, the halogenated ones creating major damages to the environment. One of the solutions so far has been to treat and recycle the solvents or to use them as fuel after employing them in a chemical process. A major research effort is now being made to find alternatives to the use of these

organic solvents. The challenging approach that we have chosen is to develop organic reactions in the absence of solvent by mechanochemistry.

Mechanochemical activation can be a useful tool for solvent-free organic synthesis. Designed at the beginning for crushing inorganic matter, apparatus such as ball-mills proved their efficacy in some organic chemistry reactions and can be applied on an industrial scale. We have shown that this kind of activation is applicable to the synthesis of important organic molecules, including amino acid derivatives and peptides.<sup>1</sup> In the last years, we have developed this methodology and applied it to peptides such as aspartame or enkephalin or heterocycles such as hydantoins.<sup>2</sup> More recently, in connection with other projects dedicated to green chemistry in our group, we have investigated mechanochemistry in palladium-catalyzed reactions and in the preparation of organometallic complexes.<sup>3</sup>

**References**

1. a. T.-X. Métro, E. Colacino, J. Martinez, F. Lamaty « Amino acids and Peptides in Ballmilling » in *Ball Milling Towards Green Synthesis: Applications, Projects, Challenges RSC Green Chemistry Series* 2015 p. 114-150. b. Declerck, V. ; Nun, P.; Martinez, J.; Lamaty, F. *Angew. Chem. Int. Ed.* **2009**, *48*, 9318-9321. c. Bonnamour, J.; Métro, T.-X.; Martinez, J.; Lamaty, F. *Green Chem.* **2013**, *15*, 1116-1120. d. Métro, T.-X.; Bonnamour, J.; Reidon, T.; Duprez, A.; Sarpoulet, J.; Martinez, J.; Lamaty, F. *Chem. Eur. J.* **2015**, *21*, 12787-12796. e. V. Porte, M. Thioly, T. Pigoux, T.-X. Métro, J. Martinez, F. Lamaty *Eur. J. Org. Chem.* **2016**, 3505-3508
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3. a. V. Declerck, E. Colacino, X. Bantreil, J. Martinez, F. Lamaty, *Chem. Commun.* **2012**, *48*, 11778-11780. b. Beillard, A.; Golliard, E.; Gillet, V.; Bantreil, X.; Métro, T.-X.; Martinez, J.; Lamaty, F. *Chem. Eur. J.* **2015**, *21*, 17614-17617 c. Beillard, A.; Bantreil, X.; Métro, T.-X.; Martinez, J.; Lamaty, F. *Chem. Sci.* in print

**Date:** October 24, 2016 (Monday)

**Time:** 4:30 p.m.

**Venue:** LT3, Lady Shaw Building



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Contact Person:  
Prof. Zuowei Xie



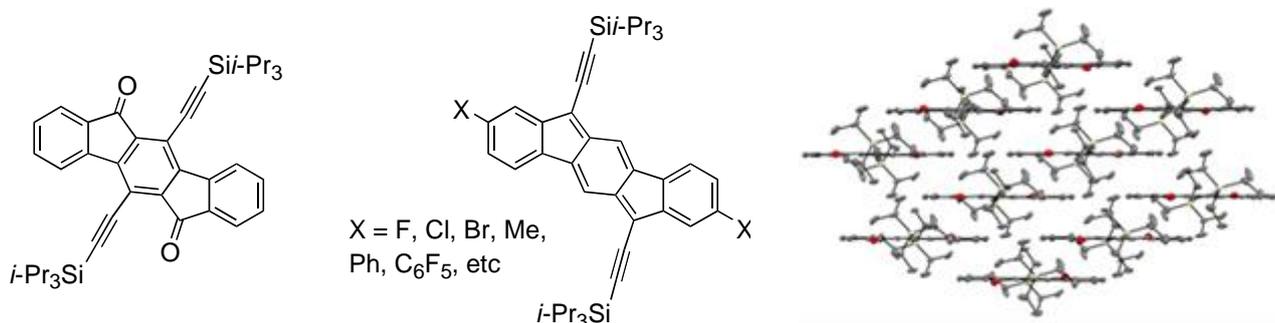
*The Chinese University of Hong Kong*  
*Department of Chemistry*  
*Research Seminar Series*

**Speaker:** Prof. Michael M. Haley  
 Department of Chemistry & Biochemistry  
 University of Oregon

**Title:** Indenofluorenes and Ring-Expanded Analogues: From Quinoidal Electron-Accepting Materials to Stable Organic Biradicals

<< Abstract >>

This talk will present our synthetic, structural and materials studies of a new class of electron-accepting molecules based on the indenofluorene (IF) skeleton. The initial preparative route involved transannular cyclization of octadehydrodibenzo[12]annulenes to afford the pentacyclic ring system. Subsequent transformations generated the first stable examples of the fully conjugated, 20 pi-electron, formally anti-aromatic compounds. Optimization of intermediate IF-6,12-dione synthesis via a simple three-step process now permits access to IF derivatives in multigram quantities. Work on 6,12-diaryliIFs demonstrated that single crystals of the pentafluorophenyl derivative could serve as an active layer in organic field effect transistors (OFETs) that exhibit ambipolar behavior using Au source/drain contacts. Current studies are focused on replacing the benzene groups with thiophene units as well as expanding the quinoidal core. This presentation will focus on development of project as well as include the latest results from our lab.



**Date:** October 31, 2016 (Monday)

**Time:** 4:30 p.m.

**Venue:** LT3, Lady Shaw Building



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Contact Person:  
Prof. Qian Miao