For favour of posting

The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series
（普通話主講）

Speaker: 劉雲圻教授
中國科學院化學研究所

Title: 分子材料与器件

分子材料是通過分子間弱相互作用（如氫鍵、π–π相互作用、范德華力等）而形成的材料。與傳統的由化學鍵而形成的矽基、化合物半導體材料不同，分子材料一般為長程無序的無定形和多晶材料；導電的載流子除電子和空穴外，還有質子、離子、極化子和孤子；導電機理被認為是“跳躍”機理而非能帶導電。分子材料與器件的主要優點是光電性能可通過分子設計來調控，種類多，可溶液法加工，器件具有柔性，大面積和低成本。而主要缺點是穩定性比較差，光電器件性能有待提高。分子材料在有機場效應電晶體、有機發光二極體、有機太陽能電池和感測器等方面具有廣泛的應用前景。

本報告將介紹π–共軛有機小分子/高分子和石墨烯材料的設計、合成，和電性能研究，主要集中在場效應電晶體方面。

Date: January 3, 2017 (Tuesday)

Time: 10:30 a.m.

Venue: L3
Science Centre

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Contact Person:
Prof. Zuowei Xie

For favour of posting

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

Speaker: Prof. Jinming Gao
Professor of Oncology, Pharmacology, and Otolaryngology
UT Southwestern Medical Center
U.S.A.

Title: pH Transistor Nanomedicine

Date: January 4, 2017 (Wednesday)

Time: 10:30 a.m.

Venue: L3
Science Centre

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Contact Person:
Prof. Chi Wu

For favour of posting

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

Speaker: Prof. Lizhu Wu
Director of the Lab of Supramolecular Photochemistry
Technical Institute of Physics and Chemistry
Chinese Academy of Science (CAS)

Title: Artificial Photosynthetic Systems for Chemical Transformation

Date: January 6, 2017 (Friday)

Time: 4:30 p.m.

Venue: L1
Science Centre

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Contact Person:
Prof. Zuowei Xie

For favour of posting

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

Speaker: Prof. Shou-Fei Zhu
Professor of Chemistry
Nankai University

Title: Catalytic Hydrogen Transfer Reactions

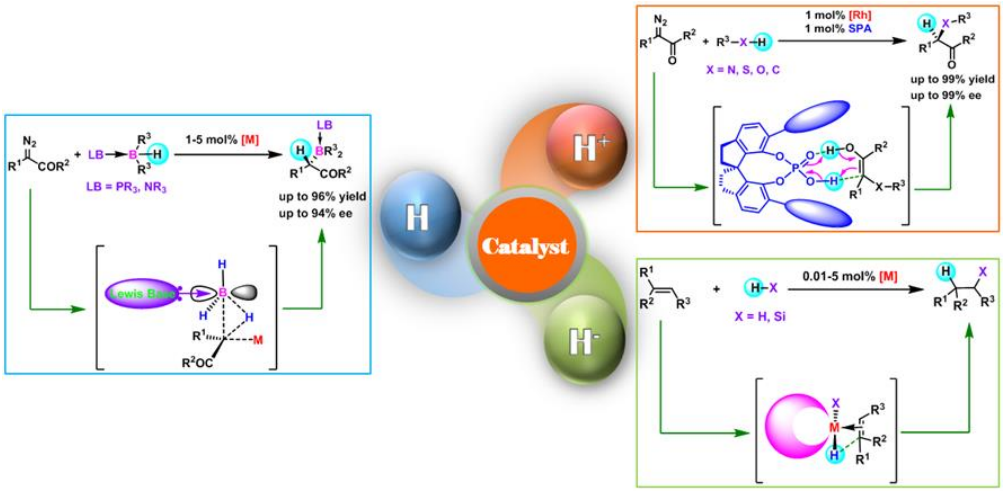
Date: January 13, 2017 (Friday)

Time: 2:30 p.m.

Venue: LT2, Lady Shaw Building

< Abstract >

The hydrogen transfer processes are ubiquitous in catalytic organic reactions and many of them involving in the rate-determined or selectivity-determined steps. The development of efficient catalysts to control of hydrogen transfer steps in organic reactions is of critical for improving their efficiency but is still a significant challenge nowadays. In this talk, I will report our recent progresses on the development of new catalysts for organic reactions involving hydrogen transfer as key steps: 1, the development of novel "chiral proton shuttle" catalysts for metal-catalyzed reactions, which can realize efficient chiral control of proton transfer of active intermediates and have been recognized as "an area poised for further development"; 2, the development of a new catalytic B–H bond insertion reaction, which contains a critical hydrogen atom transfer process and provide "an attractive approach to chiral organoborons"; 3, the development of efficient transition-metal catalysts for the hydrogenation and hydrosilylation, which contain metal-hydride transfers as key steps and have been used for preparing functional compounds.



Prof. Shou-Fei Zhu is a professor of chemistry at Nankai University, Tianjin, China. He obtained his PhD from Nankai University in chemistry in 2005 (Mentor: Qi-Lin Zhou) and did his postdoctoral work in the department of chemistry at the University of Tokyo (Mentor: Prof. Eiichi Nakamura). He had been a lecture (2005–2008) and associate professor (2008–2013) in the Institute of Elemento-Organic Chemistry at Nankai University and promoted to a full professor from 2013 at the same institute. His research interests focus on catalytic organic synthesis, particularly on the asymmetric catalysis. He authored 80 peer-reviewed research papers, 2 chapters on the scientific books, and 6 patents. He is supporting by several talent programs of China including National Outstanding Young Investigator of NSFC and National Program for Support of Top-notch Young Professionals. He won several awards and honors including Young Chemist Award of Chinese Chemical Society and Tianjin Youth Award for Science and Technology.

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Contact Person:
Prof. Gavin C. Tsui

For favour of posting

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

Speaker: Professor Alex Edwin Bunker
Faculty of Pharmacy
University of Helsinki

Title: Computationally assisted design (CAD) for drug delivery; Molecular dynamics modelling as a tool in nanomedicine: Liposome based drug delivery systems as a case study

<< *Abstract* >>

The development of nanoscale drug delivery mechanisms, nanomedicine, is one of the most promising new avenues for drug delivery. It carries the promise of extending the solubility profile of drugs that can be delivered, and effectively targeting the delivery to the desired tissue, thus increasing efficacy and reducing side effects. This field has so far, however, been far better at generating new publications than new approved drug therapies. Part of the cause of this is the extent to which trial and error based methodologies continue to dominate the drug development process. While several experimental techniques exist to investigate aspects of the behavior of nanoscale drug delivery mechanisms, there remain considerable gaps of knowledge. Computational molecular dynamics modelling (MD) with a model with all atom resolution has the potential to integrate these results, and allow for a rational design approach to be applied: engineering devices instead of trial and error development of drugs. We have performed a considerable amount of work using MD to gain insight into the structure and behavior of liposome based drug delivery systems (LDS). This can be seen as a case study of the potential for computational modeling to be used, alongside complementary experiments, to achieve a design based approach in nanomedicine.

Date: January 13, 2017 (Friday)

Time: 4:30 p.m.

Venue: L1, Science Centre

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Contact Person:
Prof. To Ngai

For favour of posting

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

Speaker: Prof. Gregory A. Voth
Department of Chemistry
The University of Chicago

Title: Proton Transport in Aqueous and Biomolecular Systems: A Remarkably Complex and Collective Phenomenon

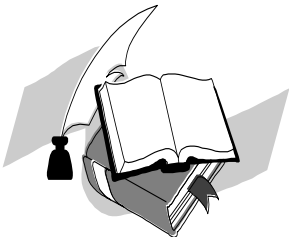
<< Abstract >>

The hydrated excess proton (aka “hydronium cation”) is critical in many areas of chemistry, biology, and materials science. Despite playing a central role in fundamental chemical (e.g., acid-base) and biological (e.g., bioenergetics) processes, the nature of the excess proton remains mysterious, surprising, and sometimes misunderstood. In this presentation our longstanding efforts to characterize proton solvation and transport in biomolecular systems will be described. These studies employ a novel, accurate, and computationally efficient multiscale reactive molecular dynamics method combined with large scale computer simulation. The methodology allows for the treatment of explicit (Grotthuss) proton shuttling and charge defect delocalization, which strongly influences proton solvation and transport in proteins such as transmembrane proton channels, pumps, and transporters/antiporters. The unique electrostatics related to the dynamic delocalization of the excess proton charge defect in water chains and amino acid residues will be elaborated, as well as the effects of these complex electrostatics on the proton transport and selectivity properties. The often opposing and asymptotic viewpoints related to electrostatics on one hand and Grotthuss proton shuttling on the other will be reconciled and unified into a single conceptual framework. The intrinsically coupled nature of the excess proton translocation and the water hydration can also be elaborated through these computer simulations. It is found that a prior existing “water wire”, e.g., one seen in an x-ray crystal structure, is not necessary for excess protons to transport through hydrophobic spaces in proteins via water mediated Grotthuss shuttling. The proton translocation process can sometimes create its own transient water wire as needed. Specific simulation results will be given for the M2 proton channel in influenza A, the proton pump cytochrome c oxidase (CcO), and the ClC Cl-/H+ antiporter. A comparison to experimental results will also be provided.

Date: January 20, 2017 (Friday)

Time: 4:30 p.m.

Venue: L1, Science Centre



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Contact Person:
Prof. Steve Y.L. Tse