

The Chinese University of Hong Kong Department of Chemistry

Research Seminar Series

Speaker: Professor Hiroshi Watanabe

Division of Multidisciplinary Chemistry

Institute for Chemical Research

Kyoto University

Title: Viscoelastic and Dielectric Investigation of

Entanglement Dynamics of Flexible Polymers

Date: February 6, 2018 (Tuesday)

Time: 10:30 a.m.

Venue: Room 707

Mong Man Wai Building





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

Speaker: Professor Jer-Lai Kuo

Institute of Atomic and Molecular Science

Academia Sinica

Title: Vibrational Anharmonicity and IR Spectra of Hydrogen

Bonded Clusters

<< Abstract >>

Structure of hydrate proton is typically classified into Eigen (H_3O^+) and Zundel $(H_5O_2^+)$ forms. While this is a textbook knowledge, it remains very challenging to keep track of their vibrational signatures owing to the strong vibrational coupling. We have developed several computational scheme to reveal the vibrational couplings (from strong to weak) with the hope to link vibrational spectra and the structure of these clusters. Gas-phase ionic spectra collected over the last two decades have provided plenty of experimental vibrational spectra that allow us to examine the vibrational motion of proton in H-bonded cations. In this talk, we will present our recent systematic theoretical studies both different types of Zundel^{1,2} and H_3O^+ under different solvation environments^{3,4}. Our theoretical studies engage *ab initio* treatment on a selected set of quantum degrees of freedom and treat their vibrational anharmonicity/coupling explicitly. If time permits, we will also access the performance of a few approximate treatments on vibrational coupling/anharmonicity to treat larger hydrogen-bonded molecular clusters⁵.

References

[1] J.A. Tan and J.-L. Kuo. J. Phys. Chem. A., 119, 11320 (2015)

[2] J.A. Tan and J.-L. Kuo. Phys. Chem. Chem. Phys., 18, 14531 (2016)

[3] J-W Li, M. Morita, T. Takahashi, and J-L Kuo, J. Phys. Chem. A, 119, 10887 (2015)

[4] J. Tan, J-W Li, C-c Chiu, H. Huynh, H-Y Liao, and J-L Kuo, Phys. Chem. Chem. Phys., 18, 30721 (2016)

[5] K-L Ho, L-Y Lee, M. Katada, A. Fujii, and J-L Kuo, Phys. Chem. Chem. Phys., 18, 30498 (2016)

Date: February 8, 2018 (Thursday)

Time: 2:30 p.m.

Venue: Room G06, Y.C. Liang Hall





The Chinese University of Hong Kong Department of Chemistry

Research Seminar Series

Speaker: Professor Shengming Ma (Academician)

State Key Laboratory of Organometallic

Chemistry

Shanghai Institute of Organic Chemistry, CAS

Title: Catalytic Enantioselective Synthesis of Allenes

Date: February 9, 2018 (Friday)

Time: 4:30 p.m.

Venue: L1

Science Centre









The 11th Lecture Series by Academicians from the Chinese Academy of Sciences (CAS)

Jointly Organized by
Department of Chemistry
Office of Academic Links (China)

Speaker: Prof. LI YA DONG

Division of Chemistry

Chinese Academy of Sciences 中國科學院化學部李亞棟院士

Title: Metallic Nano, Cluster, and Single Atom

Catalysis

Date: Wednesday, 28 February 2018

Time: 44 (16:30 – 18:00) 44

Venue: LT 1, Institute of Chinese Studies

Registration: http://www.cuhk.edu.hk/oalc/cas-2018/





簡歷

Prof. Yadong Li, born in 1964, received his B.S. degree in Department of Chemistry, Anhui Normal University in 1986, Ph.D degree in Department of Chemistry, University of Science and Technology of China in 1998. He joined the faculty of Department of Chemistry, Tsinghua University in 1999 as a full professor. His research interests focus on structure-, size-, and morphology-controllable synthesis of monodisperse nanocrystals as well as properties and applications of nanomaterials. Prof. Li's work has been cited over 35000 times with H-index number of 102.

Metallic Nano, Cluster, and Single Atom Catalysis

Metallic nanocrystals, clusters, and single atoms are important catalysts that have been widely used in both heterogeneous and homogeneous catalysis. It is of great significance to understand the essence and laws of catalysis for the frontier of chemistry and chemical engineering. More and more attention has been paid to the correlation of catalyst structure and catalytic properties. To date, researchers have uncovered many important factors governing the catalytic performance of nano, cluster, and single atom catalysts, including composition, shape, size, surface/interface effects and so on.

However, challenges remain in the following aspects: intrinsically what the active site or center of the catalyst is in heterogeneous catalysis; which is the key factor determining the catalytic performance: composition, structure (shape), size, interaction between catalyst and support, or surface/interface effects; whether or not the latest achievements of nanotechnology could be applied to the fundamental and applied research of catalysis, so as to improve the activity, selectivity and stability of the catalyst, and if so, how to manage; whether enzyme catalysts could be manufactured with high activity and specific selectivity in ambient conditions as enzyme in nature. Herein, we made some explorative attempts and achieved valuable results in combination with several catalysis in chemical engineering.

Language: Putonghua/English

ALL ARE WELCOME
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