



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)

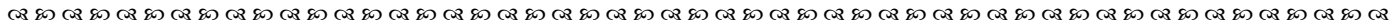
Time: 2:30 p.m.

Venue: Room G06, Y.C. Liang Hall



ALL ARE WELCOME

Contact Person:
 Prof. Zhifeng Liu



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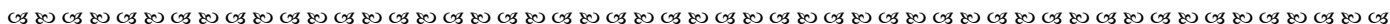
Speaker: Professor Shengming Ma (Academician)
State Key Laboratory of Organometallic
Chemistry
Shanghai Institute of Organic Chemistry, CAS

Title: Catalytic Enantioselective Synthesis of Allenes

Date: February 9, 2018 (Friday)

Time: 4:30 p.m.

Venue: L1
Science Centre



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Contact Person:
Prof. Zuowei Xie

