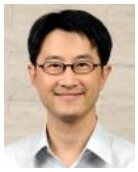
NANYANG TECHNOLOGICAL UNIVERSITY

CBC SEMINAR ANNOUNCEMENT



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Vibrational Anharmonicity and IR Spetra of Protonated Clusters

Structure of hydrate proton is typically classified into Eigen (H3O+) and Zundel (H5O2+) 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 Zundel1,2 and H3O+ under different solvation environments3,4. 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 molecular systems5.

[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:	**6th February 2017 (Monday)**
Time:	**11:00am – 12:30pm**
Venue:	**SPMS Research & Graduate Studies Office Conference Room**
Host:	**Assoc Professor Tan Howe Siang**