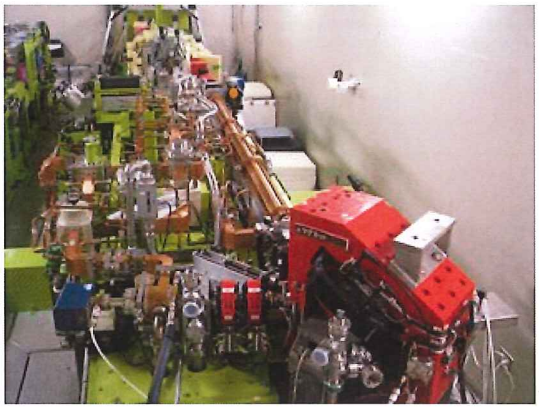
# FEL-TUS Chemical Physics Seminar



日時：平成 29 年 5 月 8 日(月)　16：30 ～ 17：30
場所：東京理科大学神楽坂キャンパス 1012 ゼミ室
講師：Dr. Jer-Lai Kuo
(Institute of Atomic and Molecular Sciences, Academia Sinica)

題目：Vibrational Anharmonicity and IR Spetra of Protonated Clusters

概要：

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 and $H_3O^+$ under different solvation environments. 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 systems.

事前登録は必要ありません。関連分野の学生・研究者の来聴を歓迎いたします。

世話人 化学科 築山光一・小山貴裕（内線 5736）