

## 講演会のお知らせ

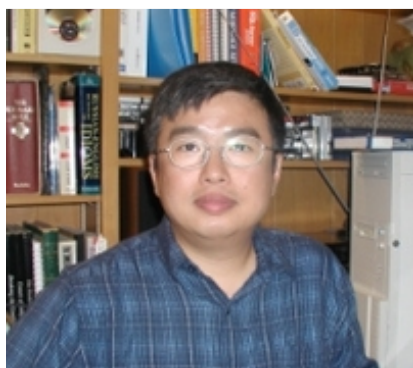
下記のとおり講演会を開催いたします。多数の御来聴をお待ち申し上げます。

### 記

- ・ 日時 : 2016年6月9日(木) 15:00
- ・ 場所 : 理学研究科B301室 (B棟)
- ・ 講演題目 : Anharmonic and damping correction on Franck–Condon factors with application to molecular electronic spectroscopy
- ・ 講演者 : Prof. Chaoyuan Zhu [National Chiao Tung University (Taiwan)]  
(朱 超原 教授 [国立交通大学(台湾)])

- ・ 概要 :

Franck–Condon factors bridge the gap between theoretical modeling and experimental observations for molecular electronic spectroscopy and electron transfer. Under the displaced harmonic oscillator approximation, multidimensional Franck–Condon factors are decomposed into a product of many one-dimensional (1D) Franck–Condon (FC) factors, and each 1D-FC factor is associated with one Huang–Rhys factor that determines the leading contribution of band shape and intensity of corresponding normal-mode vibronic spectrum. Duschinsky rotation effect and anharmonic effect may be introduced into FC factors to further improve simulation in gaseous phase. We recently developed analytical formulas of anharmonic correction in FC factors in terms of Huang–Rhys factors for modeling absorption and fluorescence spectra in gaseous phase. The analytical formulas were successfully applied to simulate absorption and fluorescence spectra for pyridine, fluorobenzene, and pyrimidine molecules and its results agree well with experimental observations. On the other hand, we developed the scaling method leading to direct modification of Huang–Rhys factors by damped oscillators for modeling absorption and fluorescence spectra in solution phase and this method was applied to perylene and rubrene molecules in solution to explain solvent-enhanced vibronic spectra.



Zhu教授は量子状態間の非断熱遷移に関する解析理論として有名な「Zhu–Nakamura理論」を構築された理論研究者で、分子科学研究所(岡崎)に勤務されたこともある“日本通”の研究者です。このたび、森野基金外国人研究者招聘により来日されたのを機に本学にお立ち寄りいただき講演を行っていただくことになりました。

(問い合わせ先)

理学研究科化学専攻反応物理化学研究グループ  
山崎 勝義

Phone & fax: 082-424-7405

E-mail: [kyam@hiroshima-u.ac.jp](mailto:kyam@hiroshima-u.ac.jp)