

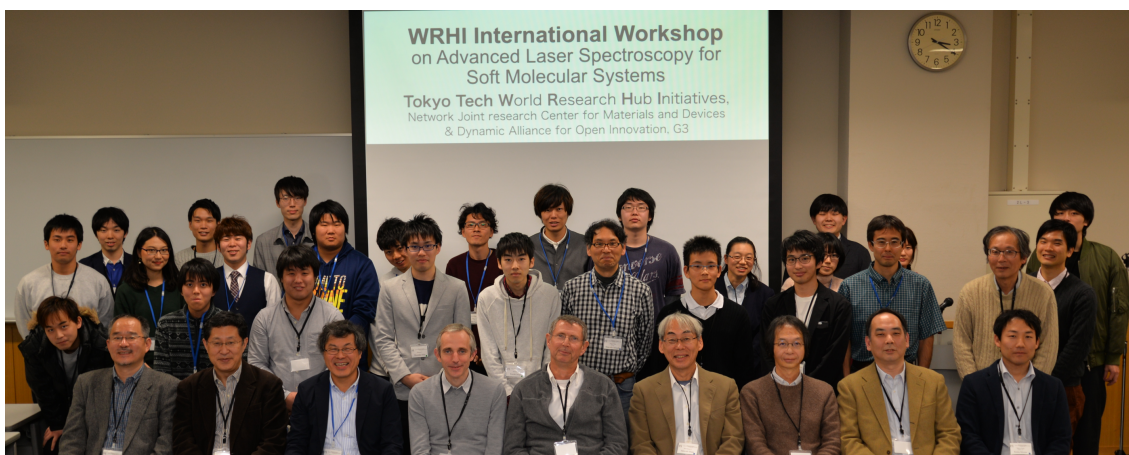
# "WRHI International Workshop on Advanced Laser Spectroscopy for Soft Molecular Systems"

Organized by

**Tokyo Tech World Research Hub Initiatives &**  
Network Joint research Center for Materials and Devices & Dynamic Alliance for  
Open Innovation, G3 Group, MEXT

30<sup>th</sup> November, 2018 @ Meeting Room #1, Suzukake Hall

The international workshop was organized for the stay of two internationally well-recognized researchers; Prof. Christophe Juvet (CNRS / U Aix-Marseille and WRHI Tokyo Tech) and Dr. Gilles Grégoire (CNRS / U Paris-Sud).



Group Photo of the Workshop

Prof. Koyama, Director-General of Institute of Innovative Research, gave opening address for the workshop.



Prof Koyama, Director-General of IIR

The first keynote lecture by Prof. Jouvét presented the new development for negative ion spectroscopy by using ESI/Cold ion trap spectrometer. The second keynote lecture by Dr. Grégoire is the photochemical processes of nuclear bases molecules, which related to photoprotection mechanism in biological systems.

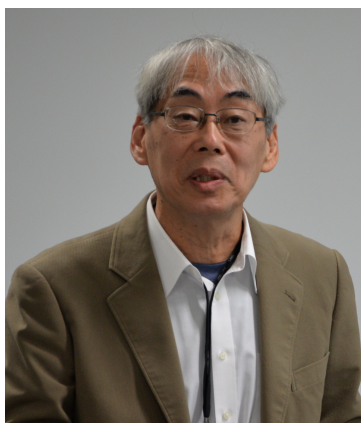


Prof. C. Jouvét



Dr. G. Grégoire

Six invited talks were presented by Japanese professors. Photochemical processes of cinnamic acid, important molecules in plants, were thoroughly revealed by Prof. Takayuki Ebata (Hiroshima U). Non-classical chemical bond formed by three electrons in one bonding ( $2c3e$ ) was found in  $(H_2S)_n$  clusters by Prof Asuka Fujii (Tohoku U). Prof Haruki Ishikawa (Kitasato U) discussed the infrared spectra of phenol-alkylsilane dihydrogen-bonded clusters.



Prof. T. Ebata



Prof. A. Fujii



Prof. H. Ishikawa



Prof Akio Kitao from School of Life Science and Technology (Tokyo Tech) presented advanced molecular dynamics on protein complex. Prof Shun-ichi Ishiuchi from Laboratory for Chemistry and Life Science (Tokyo Tech) demonstrated ion-trap laser spectroscopy on tripeptide GYG, a model system of selection filter in  $K^+$  channel, and showed origin of the ion selectivity based on the spectroscopic evidence. Dr. Kenta Mizuse from School of Science (TokyoTech) showed a beautiful rotational wave packet spectroscopy and its application on  $N_2$  dimer.



Prof. A. Kitao



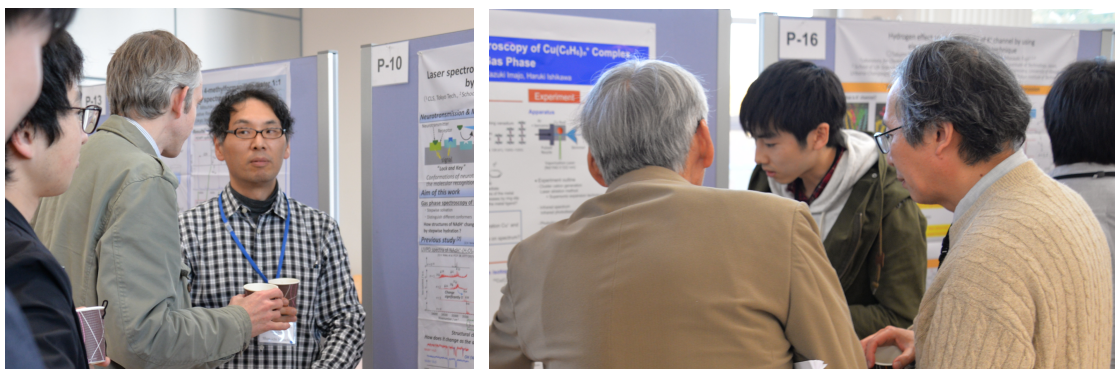
Prof. S. Ishiuchi



Dr. K. Mizuse

All the presentations were up-to-date and advanced results on soft molecular systems and 40 attendees enjoyed the intensive discussion. The workshop organized poster session for graduate students and 16 posters were presented by graduate students. It was good opportunity for students to discuss their results with top level international scientists in English. All the presentations and discussions were internationally top quality. I believe the successful workshop contributed to establish the international research hub in TokyoTech.





Poster Session

## Program

30th November, 2018

Chairperson : Masaaki Fujii

10:20 - 10:30 Opening Remarks

Fumio Koyama, (Professor, Head of WRHI, Director-General of Institute of Innovative Research (IIR), Tokyo Tech)

## Keynote Lecture 1

Chairperson : Masaaki Fujii

10:30 - 11:10 "Dissociative electron photodetachment vs. anionic photo-fragmentation of deprotonated aromatic acid"

Christophe Juvet (Aix-Marseille U)

## Invited Talks 1 ~ 2

Chairperson : Haruki Ishikawa

11:10 - 11:40 "Systematic study on nonradiative decay and photoisomerization of cinnamic acid and its derivatives"

Takayuki Ebata (Hiroshima U)

11:40 - 12:10 "High-precision rotational wave packet imaging and imaging-based spectroscopy of gas-phase molecular systems"

Kenta Mizuse (School of Science, Tokyo Tech)

12:10 - 13:30 Lunch



## **Keynote Lecture 2**

Chairperson : Takayuki Ebata

13:30 - 14:10 "Excited state dynamics of protonated DNA/RNA bases : All roads lead to the triplet state"

Gilles Grégoire (U Paris-Sud)

## **Invited Talks 3 ~ 4**

Chairperson : Mitsuhiro Miyazaki

14:10 - 14:40 "Infrared spectroscopy hemibonded clusters of H<sub>2</sub>S"

Asuka Fujii (Tohoku U)

14:40 - 15:10 "Infrared spectroscopy of Phenol-Alkylsilane dihydrogen-bonded clusters: Franck-Condon-like patterns in the OH stretch band"

Haruki Ishikawa (Kitasato U)

15:10 - 16:40 Poster Session (Lounge @ 3F, H-1 Building)

## **Invited Talks 5 ~ 6**

Chairperson : Yasuhiro Ohshima

16:40 - 17:10 "Investigating protein complex formation and dissociation in silico"

Akio Kitao (School of Life Sci & Tech, Tokyo Tech)

17:10 - 17:40 "Ion selectivity of K<sup>+</sup> channel studied by cold ion trap infrared spectroscopy"

Shun-ichi Ishiuchi (CLS, Tokyo Tech)

17:40 - 17:50 Closing Remarks (Masaaki Fujii, WRHI, CLS, IIR, Tokyo Tech)

18:00 Banquet (Lounge @ 3F, H-1 Building)

**Poster Session (15:10 - 16:40)**

- P-01 "Visualization of rotational eigenstates and wave packets of nitric oxide"

(Tokyo Tech) Dai Ikeda, Kenta Mizuse, Yasuhiro Ohshima

- P-02 "Real-time observation of intermolecular vibrational dynamics in benzene clusters"

(Tokyo Tech) Tomomi Murai, Kenta Mizuse, Hirokazu Hasegawa, Yasuhiro Ohshima

- P-03 "IR-induced structural change in the microscopic hydration of phenol cations trapped in the cold ion trap"

(Kitasato Univ.) Hikaru Sato, Yasutoshi Kasahara, Haruki Ishikawa

- P-04 "Dihydrogen bond in the electronic excited states of various phenol-alkylsilane clusters: Interaction between the OH stretching and intermolecular vibrational modes"

(Kitasato Univ., \*Shizuoka Univ.) Takutoshi Shimizu, Masaaki Uchida, Yoshiki Kigure, Yasutoshi Kasahara, Yoshiteru Matsumoto\*, Haruki Ishikawa

- P-05 "Photodissociation Spectroscopy of  $\text{Cu}(\text{C}_6\text{H}_6)_n^+$  Complex in Gas Phase"

(Kitasato Univ.) Kazuki Imajo, Haruki Ishikawa

- P-06 "Si-H...H-O type dihydrogen bond in the phenol-alkylsilane clusters: Re-investigation based on the electronic spectra"

(Kitasato Univ., \*Shizuoka Univ.) Masaaki Uchida, Takutoshi Shimizu, Yoshiki Kigure, Yasutoshi Kasahara, Yoshiteru Matsumoto\*, Haruki Ishikawa

- P-07 "Temperature dependence of the hydrogen-bond structures of cluster cations trapped in the temperature-variable ion trap"

(Kitasato Univ.) Masataka Orito, Keita Suzuki, Hikaru Sato, Yasutoshi Kasahara, Haruki Ishikawa



P-08 "Real-time observation of solvent reorientation dynamics in the (p-cyanophenyl) pentamethyldisilane-water<sub>2</sub> cluster by picosecond time-resolved spectroscopy"

(Tokyo Tech) Yuki Konno, Mitsuhiko Miyazaki, Masaaki Fujii

P-09 "Gas phase spectroscopy of hydorated clusters of protonated nicotine and nornicotine by using electrospray / cold ion trap technique"

(Tokyo Tech) Kazuya Tsuruta, Shun-ichi Ishiuchi, Sotiris S. Xantheas,  
Masaaki Fujii

P-10 "Laser spectroscopy of hydrated clusters of protonated noradrenaline by using electrospray / cold ion trap technique"

(Tokyo Tech) Keisuke Yamaguchi, Shun-ichi Ishiuchi, Masaaki Fujii

P-11 "Mid-IR spectrum of benzene dimer cation and the charge resonance state formation dynamics"

(Tokyo Tech) Remina Otsuka, Mitsuhiko Miyazaki, Masaaki Fujii

P-12 "Development of IR-IR ion dip spectroscopy for ultra-cold ions trapped in a cryogenic ion trap"

(Tokyo Tech) Kenichi Kasai, Shun-ichi Ishiuchi, Masaaki Fujii

P-13 "Ionization induced water migration in the 4-methylformanilide–water 1:1 cluster probed by IR dip spectroscopy"

(Tokyo Tech) Tairiku Kamiya, Mitsuhiko Miyazaki, Masaaki Fujii

P-14 "Structural study on a partial peptide of intrinsically disordered protein  $\alpha$ -synuclein - small ligands complexes by electrospray / cold ion trap laser spectroscopy"

(Tokyo Tech) Mizuki Tabata, Shun-ichi Ishiuchi, Masaaki Fujii

- P-15 "Gas phase spectroscopy of a partial peptide of adrenoceptor (SIVSF) - ligands complexes by electrospray / cold ion trap technique -Chiral effect on molecular recognition-"

(Tokyo Tech) Masato Tamura, Shun-ichi Ishiuchi, Masaaki Fujii

- P-16 "Hydration effect on ion selectivity of  $K^+$  channel by using electrospray cryogenic ion trap technique "

(Tokyo Tech) Takumi Negoro, Shun-ichi Ishiuchi, James M. Lisy, Masaaki Fujii