

3rd International Symposium of **JSPS Core-to-Core Program** on  
**“Molecular Recognition Mechanism between Flexible Molecules”**

*in cooperation with IRFI, iPWR & CLS IIR, TokyoTech*

*&*

*Network Joint research Center for Materials and Devices &*

*Dynamic Alliance for Open Innovation*

**Lecture Hall, S8 Bldg, Suzukakedai Campus, Tokyo Institute of Technology**

29th September, 2022

10:00 - 10:10     Opening Remarks

Masaaki Fujii, (Japanese Coordinator, Tokyo Tech)

**Keynote Lecture 1**

Chairperson :     Masaaki Fujii (TokyoTech)

10:10 - 10:50     "Geometric & Electronic Structure of Silane-Based Cation Clusters:  
Charge-Inverted H-Bonds, 3c-2e Bonds & Silicon Hydride Wires"  
**(K-1)**

Otto Dopfer (German Coordinator, TU Berlin & IRFI TokyoTech)

**Invited Talks 1 ~ 2**

Chairperson :     Yoshiteru Matsumoto (Shizuoka U)

10:50 - 11:20     "Cold ion trap spectroscopy of partial peptides of adrenalin receptor-  
ligand complexes" **(I-1)**

Shun-ichi Ishiuchi (Tokyo Tech)

11:20 - 11:50     "Searching the Structure of a Capped Pentapeptide, SIVSF, Using a  
Similarity Score of Infrared Spectra" **(I-2)**

Kiyoshi Yagi (RIKEN)

11:50 - 13:10     Lunch

## Keynote Lecture 2

Chairperson : Keisuke Hirata

13:10 - 13:50 "Conformer-selective Photodynamics of TrpH<sup>+</sup>-H<sub>2</sub>O" **(K-2)**

Gilles Grégoire (CNRS / U Paris-Saclay)

## Invited Talks 3 ~ 4

Chairperson : Keisuke Hirata

13:50 - 14:20 "Quantum-state control of molecular vibration and rotation"

Yasuhiro Ohshima (TokyoTech) **(I-3)**

14:20 - 14:50 "Theoretical Study on Solvation Clusters of NH<sub>4</sub> and H<sub>3</sub>O" **(I-4)**

Kenro Hashimoto (Open U)

14:50 - 16:10 Group Photo & Poster Session

## Keynote Lecture 3

Chairperson : Shun-ichi Ishiuchi (TokyoTech)

16:10 - 16:50 "Computational Studies of the Infrared Spectra of Hydrogen Bonding Networks Consisting of Inter- and Intra-molecular Hydrogen Bonds" **(K-3)**

Sotiris Xantheas (PNNL / Washington U)

## Invited Talks 5 ~ 6

Chairperson : Kenta Mizuse (Kitasato U)

16:50 - 17:20 "Dynamical behavior of hydrogen-bonded phenol cations in the cold ion trap" **(I-5)**

Haruki Ishikawa (Kitasato U)

17:20 - 17:50 "Observation of Ar Migration in the 4-Aminobenzonitrile–Ar Cluster by MATI-IR Spectroscopy" **(I-6)**

Mitsuhiko Miyazaki (Ochanomizu U)

17:50 - 18:00 Closing Remarks

Michito Yoshizawa, (CLS, IIR, Tokyo Tech)