

International Symposium of JSPS Core-to-Core Program

Coorganized by

Chemistry and Life Science Laboratory (ILR, Tokyo Tech) & The Cooperative Research Program "Network Joint Research Center for Materials and Devices" (MEXT),

29th July – 2nd August 2024,

29th -30th July @ Tokyo Institute of Technology (Ookayama, Tokyo: Main symposium)

31st July – 1st August @ Hotel Belnatio (Niigata: Satellite meeting)

2nd August @ Tokyo Institute of Technology / Chuo University (Collaboration Discussion)

Part 1 : Final Symposium in Japan

7th International Symposium of JSPS Core-to-Core Program on "*Molecular Recognition Mechanism between Flexible Molecules*"

Program 29th July, 2024

---- Session Chair: Masaaki Fujii (TokyoTech) ----

10:30

Opening Remarks

Michito Yoshizawa, *Japanese Coordinator* (Tokyo Tech)

10:40 (O1)

"Spectroscopy and Dynamics of Ions and Cluster Ions"

Otto Dopfer (TU Berlin)

11:10 (C1)

"Intermolecular dynamics in molecular clusters probed by real-time wave packet imaging"

Kenta Mizuse (Kitasato U)

11:30 (C2)

"Hydrated structures of the charge-resonance pyrrole dimer cation studied by IR spectroscopy",

Yoshiteru Matsumoto (Shizuoka U)

11:50 (C3)

"Alkyl-Aromatic Hybrid Micelles"

Michito Yoshizawa (Tokyo Tech)

12:10 Lunch

---- Session Chair: Haruki Ishikawa (Kitasato U) ----

13:40 (O2)

"Conformer-selective spectroscopic studies of chiral molecules : from structure to chiroptical spectroscopy"

Anne Zehnacker-Rentien (CNRS / U. Paris-Saclay)

14:10 (O3)

“Vibrational mode-dependent circular dichroism spectroscopy of gas-phase molecules”,
Nam Joon Kim (Chungbuk U)

14:40 (C4)

“Conformational dynamics and function of membrane proteins regulated by ligand binding”

Akio Kitao (Tokyo Tech)

15:00 (C5)

“IR spectroscopy at a single vibrational level in cationic states by MATI-IR spectroscopy - possibility of Ar migration in the resorcinol–Arn (n = 1, 2) clusters--”

Mitsuhiko Miyazaki (Ochanomizu U)

15:20 Coffee break

---- **Session Chair: Yoshiteru Matsumoto (Shizuoka U)** ----

15:50 (O4)

“First-principle exploration on the conformational space of peptides and saccharides assisted by neural network potential”

Jer-Lai Kuo (*IAMS, Academia Sinica*)

16:20 (C6)

“An old but new approach to hydrogen bond energy determination: Revisit to the Badger-Bauer rule with gas phase protonated clusters”,

Asuka Fujii (Tohoku U)

16:40 (O5)

“Tyrosine Nitration: Insights from Isomeric Structures”,

Ivan Chu (U Hong Kong)

17:10 (C7)

“Isomer separation of reaction intermediates and products by ion mobility-mass spectrometry”

Fuminori Misaizu (Tohoku U)

17:30 (C8)

“Multiple Proton/Hydrogen Transfer in 7-Azaindole–S_n and 7-Hydroxyquinoline–S_n (S=H₂O, CH₃OH, NH₃) Clusters”

Hiroshi Sekiya (Kyushu U)

17:50

Closing Remarks

Otto Dopfer, *German coordinator* (TU Berlin)

18:00 End of Session

18:30 Invited Speakers' Dinner (Invited speakers and organizers only)

Part 2 : Kick-Off Symposium

1st International Symposium of JSPS Core-to-Core Program on *“Elucidation of solvation effects on molecular recognition”*

Program 30th July, 2024

---- Session Chair: Shun-ichi Ishiuchi (Tokyo Tech) ----

10:00

Opening Remarks 1

Japanese Coordinator, Shun-ichi Ishiuchi (Tokyo Tech)

10:10

Opening Remarks 2

USA Coordinator, Sotiris S. Xantheas (PNNL)

10:15 (O6)

“Switching of protonation sites in hydrated nicotine via a Grotthuss mechanism”

Sotiris S. Xantheas (PNNL)

10:45 (C9)

“Probing proton transfer mechanisms in hydrated clusters by cryogenic double ion trap spectroscopy”

Keisuke Hirata (Tokyo Tech)

11:05 (O7)

“Dynamics of excited state proton transfer”

Mattanjah de Vries (UC Santa Barbara)

11:35 (O8)

“Using Path Integral Methods to Understand Nuclear Quantum Effects in Hydrogen Bonded Systems”

Britta A. Johnson (PNNL)

12:05 Conference Photo, Lunch break & poster session

---- Session Chair: Kenta Mizuse (Kitasato U) ----

14:00 (O9)

“Photoelectron spectroscopy of micro-solvated clusters and host–guest anionic complexes”

Xue-bin Wang (PNNL)

14:30 (C10)

“Pyrazine: A Multi-Generational Exploration”

Toshinori Suzuki (Kyoto U)

14:50 (O10)

“Cryogenic Ion Spectroscopy to Locate the Phosphorylation Sites in a Tryptic Peptide of a Kinase Domain”

Hyuk Kang (Ajou U)

---- Session Chair: Tomohisa Sawada (Tokyo Tech) ----

15:10 (H1)

“Metal-induced folding and assembly of short peptides”

Tomohisa Sawada (Tokyo Tech)

15:25 (H2)

“Synthesis of self-assembled architectures in both solution and solid state based on intermolecular interactions”

Masahiro Yamashina (Tokyo Tech)

15:40 (H3)

“Elucidation of Reactivity of Sulfenyl Iodides Utilizing Molecular Cavities”

Satoru Kuwano (Tokyo Tech)

15:55 Coffee break

---- Session Chair: Mitsuhiro Miyazaki (Ochanomizu U) ----

16:30 (O11)

“Revisiting step-wise hydration of M^+ (18-Crown-6) complexes: Probing the etheric ring vibrational modes to unbuckle the mechanism behind size-selectivity”

James M. Lisy (Illinois U)

17:00 (C11)

“Cold Gas-Phase Spectroscopy of Chemical Intermediates Formed in Solutions”

Yoshiya Inokuchi (Hiroshima U)

17:20 (C12)

“Hydrogen bonding with cycloalkanes as proton acceptors”

Haruki Ishikawa (Kitasato U)

17:40 (C13)

“Development of Charge Carrier-Selective Heterodyne Transient Grating Spectroscopic Technique and Its Application in the Distinction of Surface Trap States in Hematite”

Woon Yong Sohn (Chungbuk U)

18:00

Closing Remarks

French Coordinator, Anne Zehnacker (CNRS / U. Paris-Saclay)

18:10 End of Session

18:30 Banquet

Program 31st July, 2024

[Moving to the Satellite Meeting Venue \(Niigata, Hotel Belnatio\)](#)

[13:00-16:00 Satellite Meeting on International Collaborations,](#)

[20:00-22:00 Free Discussion](#)

Program 1st August, 2024

[9:00-11:00 Discussion on International Collaborations](#)

[Return to Tokyo / Yokohama](#)

Program 2nd August, 2024

[Free Discussion on international collaborations / Lab tour \(Ishiuchi's lab etc\)](#)