

“Symposium on Molecular Science and Synthesis of Functional Molecules for Next Generation”, March 10 and 11, 2014

Program

March 10 (Mon.)

08:45-08:55 Opening remark (Prof. T. Ebata)

Chairperson : T. Ebata

08:55-09:40 **S-1** Prof. Thomas R. Rizzo, École Polytechnique Fédérale de Lausanne

Plenary lecture (Morino Lecture)

“New Dimensions in the Spectroscopy of Biomolecular Ions”

09:40-10:10 **O-1** Prof. Yoshiya Inokuchi, Hiroshima University

“Cold Ion Spectroscopy of Host-Guest Complexes in the Gas Phase”

10:10-10:40 **O-2** Dr. Shun-ichi Ishiuchi, Tokyo Institute of Technology

“Gas-phase spectroscopy of small peptides - conformation vs excited state dynamics”

10:40-10:50 Coffee break (Restaurant La Boheme, 1st Floor)

Chairperson : Y. Inokuchi

10:50-11:20 **O-3** Dr. Ryoji Kusaka, Hiroshima University

“Single-conformation spectroscopy of synthetic peptide foldamers”

11:20-11:50 **O-4** Prof. Asuka Fujii, Tohoku University

“Infrared spectroscopy of methanol: A cluster study on hydrogen bond structures”

11:50-12:20 **O-5** Dr. Shoichi Yamaguchi, Riken

“Heterodyne-Detected SFG Spectroscopy for Liquid Interfaces”

12:20-13:30 Lunch (Restaurant La Boheme, 1st Floor)

Chairperson : K. Inoue

13:30-14:10 **S-2** Prof. Leroy Cronin, University of Glasgow

“Explaining the Self Assembly of Gigantic Molecular Structures”

14:10-14:30 **O-6** Prof. Sadafumi Nishihara, Hiroshima University

“Development And Applications Of Ion Motion System In Solid”

14:30-15:00 **O-7** Prof. Masayuki Takeuchi, National Institute for Materials Science

“Supramolecular Approach toward Functional Organic Materials”

15:00-15:20 Coffee break (Restaurant La Boheme, 1st Floor)

Chairperson : T. Haino

15:20-15:50 **O-8** Prof. Takayoshi Nakamura, Hokkaido University

“Dielectrics based on Supramolecular Rotator Units in Single Crystals”

15:50-16:20 **O-9** Prof. Takashi Kato, University of Tokyo
“Development of Functional Molecular Assemblies”

16:20-16:50 **O-10** Prof. Kimihisa Yamamoto, Tokyo Institute of Technology
“Fine-controlled Metal-assembling Using a Dendrimer Reactor”

16:50-17:30 **S-3** Prof. Pablo Ballester, Institute of Chemical Research of Catalonia (ICIQ)
“Assembly of dimeric capsules with polar interiors”

17:30-18:50 Poster session (2nd Floor)

19:00-21:00 Banquet (Saijo HAKUWA HOTEL)

March 11 (Tue.)

Chairperson : S. Nishihara

09:00-09:30 **O-11** Prof. Shin Aoki, Tokyo University of Science
“Design and Synthesis of Photochemically and Biologically Active Iridium Complexes for Cell Imaging and Induction of Cell Death”

09:30-10:00 **O-12** Prof. Hiroki Oshio, University of Tsukuba
“Metal Complexes with Multi-bistability”

10:00-10:30 **O-13** Prof. Atsushi Nakajima, Keio University
“Electronic properties of size-selected nanoclusters landed onto alkanethiolate self-assembled monolayers”

10:30-10:50 Coffee break (Restaurant La Boheme, 1st Floor)

Chairperson : M. Aida

10:50-11:30 **S-4** Dr. Sotiris S. Xantheas, Pacific Northwest National Laboratory
“Guest / host interactions in clathrate hydrates: from model systems to periodic lattices”

11:30-11:50 **O-14** Dr. Dai Akase, Hiroshima University
“Intra- and intermolecular interactions of α -, β -, γ -cyclodextrins: from the gas phase to aqueous solution”

11:50-13:10 **O-15** Dr. Tomoki Yoshida, Hiroshima University
“Theoretical study on isomers and conformational barriers of gas phase nicotine, nornicotine and their protonated forms”

12:10-13:00 Lunch (Restaurant La Boheme, 1st Floor)

Chairperson : T. Yoshida

13:00-13:30 **O-16** Prof. Junya Hasegawa, Hokkaido University
“Molecular excited states in proteins and solutions: a theoretical study on molecular interactions”

13:30-14:00 **O-17** Prof. Yasuteru Shigeta, Osaka University

“Theoretical Studies on Reaction Mechanism of An Enzyme Cleaving Unnatural Amide Compound”

14:00-14:30 **O-18** Prof. Kazuo Kitaura, Kobe University

“Quantum Mechanical Calculation of Proteins Using the Fragment Molecular Orbital Method ”

14:30-14:40 Concluding remark (Prof. T. Haino)

Poster Session (March 10, 17:30-18:50)

P-1 Tsugunosuke Masubuchi, Takeshi Iwasa, Atsushi Nakajima

“Photoelectron spectroscopy of $V_nBz_m^-$ cluster anions ($m = n, n \pm 1$)”

P-2 Mridula Guin, Surajit Maity, Aniket Kundu, G. Naresh Patwari

“N-Heteroaromatics: A Recipe for π -Stacking”

P-3 Fumiya Morishima, Yoshiya Inokuchi, Takayuki Ebata.

“Conformational preference in the $18C6 \cdots$ benzenediol complexes”

P-4 Kazuki Soga, Takayuki Ebata, Yoshiya Inokuchi

“Development of laser spectroscopy for cold encapsulated ion complexes in gas phase”

P-5 Takamasa Ikeda, Kenji Sakoa, Shohei Nakata, and Hiroshi Sekiya

“Hydrogen bond fluctuation in the gas phase: Infrared spectra of hydrated aryl alcohol cluster cations”

P-6 Yasunori Miyazaki, Kanji Yamamoto, Jun Aoki, Yoshiya Inokuchi, Takayuki Ebata, Masahiro Ehara

“Excited-State Dynamics of Methyl Cinnamate Derivatives”

P-7 Toshiaki Ikeda, Midori Takayama, Takeharu Haino

“Helical self-assembly and circularly polarized luminescence of platinum(II) complexes possessing phenylisoxazolybenzene units”

P-8 Ryo Sekiya, Yuichiro Uemura, Takeharu Haino

“Synthesis and Luminescence Properties of Edge-functionalized Graphene Quantum Dots”

P-9 K. Maryunina, Sadafumi Nishihara, Katsuya Inoue, G. Romanenko, A. Bogomyakov, V. Ovcharenko

“Ways of Chemical and Physical Influence on Spin-Transition-Like Phenomenon in Cu(II)-Nitroxide Complexes”

P-10 N. Artiukhova, E. Tretyakov, K. Maryunina, G. Romanenk, A. Polushkin, A. Bogomyakov, V. Ovcharenko

“Spirocyclical Derivatives of Nitronylnitroxides in Design of Cu(II)-Heterospin Complexes Manifesting Magnetic Anomaly”

P-11 Suehiro Iwata

“Analysis of Hydrogen Bond Energy and Hydrogen Bond Network in $(H_2O)_n$ ($n \leq 25$) by the Charge-Transfer and Dispersion Terms”

P-12 Ami Kosaka, Sakiko Idei, Yukiteru Katsumoto, Misako Aida

“Anomerization of glucopyranose and mannopyranose in aqueous solution studied by NMR spectroscopy”

P-13 Sakiko Idei, Misako Aida

“A Theoretical study of the hydration effect on hexopyranoses”

P-14 Hideo Doi, Yudai Watanabe, Misako Aida

“A Theoretical study of the hydration around Trimethylamine N-oxide (TMAO)”