



6th International Symposium of JSPS Core-to-Core Program on “*Molecular Recognition Mechanism between Flexible Molecules*”

16th – 20th October 2023, TU Berlin

Program 16th October, 2023

14:00–16:00 Laboratory tour @ Fritz Haber Institute Berlin (FHI Berlin)

Program 17th October, 2023

---- Session Chair: Otto Dopfer (TU Berlin) ----

9:45 Opening Remarks by German Coordinator, Otto Dopfer (TU Berlin)

10:00 *Hydration effects upon ion selectivity of crown ethers studied by cold ion trap IR spectroscopy* **(O1)**

Shun-ichi Ishuichi (Tokyo Tech)

10:30 *Induced Photoelectron Circular Dichroism onto an achiral chromophore* **(O2)**

Anne-Zehnacker (U Paris)

11:00 *Dynamical behavior of hydrated phenol cations in the cold ion trap: Structural changes in cooling processes* **(O3)**

Haruki Ishikawa (U Kitasato)

11:30 *Wave-Packet Manipulation of Large-Amplitude Motions in Flexible Molecules and Clusters* **(O4)**

Yasuhiro Ohshima (Tokyo Tech)

12:00 **Lunch break & poster session**

---- Session Chair: Masaaki Fujii (Tokyo Tech) ----

14:00 *Joining Microfluidics with IRPD Spectroscopy: Isomer- and Enantiomer-Specific Monitoring of Reaction Intermediates (O5)*

Knut Asmis (U Leipzig)

14:30 *The Back Door to the Surface Hydrated Electron (O6)*

Sotiris Xantheas (PNNL)

15:00 *Vibrational and electronic spectra of protonated vanillin: Exploring protonation sites and isomerization (O7)*

Jennifer Noble (U Marseille)

15:30 Coffee break

16:00 *Cryogenic IR and UV spectroscopy of isomer-selected cytosine radical cation (O8)*

Gilles Gregoire (U Paris)

16:30 *High Resolution Photoelectron Spectroscopy of Vibrationally Excited Anions (O9)*

Dan Neumark (U Berkeley)

17:00 *Characterization of Pyrrole Dimer Cations and Their Solvated Clusters by IR Spectroscopy (O10)*

Dashjargal Arildii (TU Berlin)

17:20 *Hydration switching on the intermolecular orientation of pyrrole dimer cations probed by IR photodissociation spectroscopy (O11)*

Yoshiteru Matsumoto (U Shizuoka)

17:40 *Photodissociation & Optical Absorption Properties of Small Silicon-Containing Clusters (O12)*

Taarna Studemund (TU Berlin)

18:10 end of session

free evening

Program 18th October, 2023

---- Session Chair: Christophe Jouvét (U Marseille) ----

10:00 *Aromatic Micelles as Water-solubilizing Nanotools for Polymers and Metal-complexes (O13)*
Mitchio Yoshizawa (Tokyo Tech)

10:30 *Conformational Change and Association/Dissociation of Proteins investigated by Parallel Cascade Selection Molecular Dynamics (O14)*
Akio Kitao (Tokyo Tech)

11:00 *Ultraviolet Photodissociation Spectroscopy of Urotropine⁺ in a Cryogenic Trap (O15)*
Parker Crandall (TU Berlin)

11:30 *High-resolution, broad-bandwidth spectroscopy of molecular clusters by real-time wave packet imaging (O16)*
Kenta Mizuse (U Kitasato)

12:00 **Lunch break & poster session**
 Conference photo

---- Session Chair: Klaus Müller-Dethlefs (U Manchester) ----

14:00 *Hydrogen Bonding with Hydridic Hydrogen – Experimental Low-Temperature IR and Computational Study: Is A Revised Definition of Hydrogen Bonding Appropriate? (O17)*
Pavel Hobza (Czech Academy of Science)

14:30 *Spectroscopy of Mass/Charge Selected Cations and Anions in Helium Droplets (O18)*
Gert von Helden (FHI Berlin)

15:00 *Ion Mobility Spectrometry and Gas-Phase Spectroscopy of Sugars (O19)*
Kevin Pagel (FU Berlin)

15:30 **Coffee break**

16:00 *Heme ligation in the gas phase (O20)*
Satchin Soorkia (U Paris)

16:30 *Vibrational spectroscopy of diamondoid cations: Solvation and Cage-Opening (O21)*
Martin George (TU Berlin)

17:00 *Two-photons Conformer specific Photoelectron Circular Dichroism (PECD) (O22)*
Etienne Rouquet (U Paris)

17:20 *Noncovalent Interactions: A brief summary of achievements*

Klaus-Müller-Dethlefs (U Manchester)

17:40 *Concluding Remarks*

Masaaki Fujii (Tokyo Tech)

19:00 Conference Dinner at 12 Apostoli Charlottenburg

Program 19th and 20th October, 2023

Laboratory tours @ TU Berlin

Discussion on collaboration projects