

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

26<sup>th</sup> October 2021, via Zoom (Oral) and Spatial Chat (Poster)

Session time: 9:00 – 12:00 (CET) = 16:00 – 19:00 (JST)

## Program

### Oral Session (Zoom)

<https://us06web.zoom.us/j/81589561230?pwd=Z04wOE1mdkZLeXFmZXptYndWMFZwUT09>

Meeting ID: 815 8956 1230, pwd: 298938

9:00 (16:00) Opening Remarks by J. Coordinator, Masaaki Fujii (TokyoTech)

9:05 (16:05) G. Coordinator's Overview and “Charge Resonance Interaction in Aromatic Clusters” **(O1)**

Otto Dopfer (TU Berlin)

9:20 (16:20) “Optical Properties of Gold Cations” **(O2)**

Marko Förstel (TU Berlin)

9:25 (16:25) “Excimer Formation Dynamics in Tetracene Dimer” **(O3)**

Roland Mitric (U. Würzburg)

9:30 (16:30) F. Coordinator's Overview and “Spectroscopic Studies of Chirality” **(O4)**

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

9:45 (16:45) “Intersystem Crossing in competition in protonated uracil” **(O5)**

Gilles Grégoire (CNRS / U. Paris-Saclay)

9:50 (16:50) “NH $\cdots$ X interactions stabilize intra-residue C5 hydrogen bonded conformations in heterocyclic  $\alpha$ -amino acid derivatives” **(O6)**

Michel Mons (CEA / U. Paris-Saclay)

9:53 (16:53) “Conformational analysis by UV laser spectroscopy : how to use internal electric fields to characterize molecular structure” **(O7)**

Eric Gloaguen (CNRS / U. Paris-Saclay)

9:58 (16:58) "Excited states computation of models of phenylalanine protein chains: Performances of the TD-DFT and CC2 methods." **(O8)**

Valérie Brenner (CEA Saclay)

10:01 (17:01) "Study of the electronic spectra and excited state dynamics of aromatic molecules in various charge states" **(O9)**

Jennifer Noble (U. Aix-Marseille)

10:06 (17:06) "Development of polyaromatic capsules as functional nanoflasks" **(O10)**

Michito Yoshizawa (TokyoTech)

10:11 (17:11) "Molecular recognition of lectin using carbohydrate-modified peptide phage libraries" **(O11)**

Hiroshi Tsutsumi (TokyoTech)

10:16 (17:16) "Observing biomolecules through a lens of computer simulation" **(O12)**

Akio Kitao (TokyoTech) (Presenter: Duy Phuoc Tran)

10:21 (17:21) "Binding, intermolecular vibration, and coherent dynamics of flexible molecular systems" **(O13)**

Yasuhiro Ohshima (TokyoTech)

10:26 (17:26) "Rotational wave packet imaging of molecular clusters and chiral molecules" **(O14)**

Kenta Mizuse (Kitasato U)

10:31 (17:31) "Temperature effect on microscopic hydrogen-bond structures of phenol cations trapped in the temperature-variable ion trap" **(O15)**

Haruki Ishikawa (Kitasato U)

10:36 (17:36) "Cold ion trap spectroscopy of complex systems in Tokyo Tech" **(O16)**

Shun-ichi Ishiuchi (TokyoTech)

10:41 (17:41) Remarks & **Group Photo** (Screen shot in Zoom)

10:50 (17:50) **Poster Session** (Spatial Chat: no pwd)

<https://spatial.chat/s/C2C-FUJII>

12:00 (19:00) **Informal Meeting** for Senior and Junior Researchers (Spatial Chat)