

Report of 8th Core-to-Core International Symposium on Ionization Induced Switching

University of Manchester, Manchester, England, 13th and 16th Dec. 2013

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The 8th symposium of the Core-to-Core program was held at Photon Science Institute (PSI) of University of Manchester on 13th and 16th Dec. 2013. The symposium intended to discuss recent progress of switch in intermolecular interactions and to give a chance for young students to present their research topics. Detailed program of the symposium can be seen in another web page (<http://www.res.titech.ac.jp/~kiso/CoreToCore/seminar.html>).

On the first day, we had a poster session at the seminar room in PSI. Taking tea and some meals, we discussed about our recent researches under relaxed atmosphere. We made new connections among the attendees through the discussion. After the poster session, we had a laboratory tour in PSI. Mr. François Michels who is a student in University of Manchester introduced the special mass spectrometer for ultracold Rydberg plasma experiment. Prof. Andrew Murray introduced the original instrument to measure the electron collisions with cold atoms. Thanks to their kind introduction, we got to know about photochemistry of cold molecules.

On the second day, we had an oral session at Lovett Lecture Theatre, Alan Turing Building. After an opening remark by prof. Klaus Müller-Dethlefs in University of Manchester who was the host of this time symposium, prof. Pavel Hobza from IOCB AS CR, Palacký U, Czech presented about the comparison of theoretical and experimental binding energy (D_0) of some noncovalent systems. He performed vibrational analysis including anharmonicity of potential energy surface based on high level coupled cluster theory upto CCSDTQ(P). He demonstrated that the theoretical values obtained by such a high level calculation accurately agree with the experimental D_0 . The resulting potential energy surface can be useful not only for the prediction of D_0 but also as a benchmark set for parameterization of DFT, which can provide less-expensive way to study larger complexes with weak interactions.

We had another two sessions in the morning. In the second session, several researchers introduced progress of their works that strongly related to interaction switch, which is the main theme of the Core-to-Core program, such as phenol–Ar, monohydrated phenyl ethanol and benzyl alcohol cations. As for phenol–Ar, a challenge of MATI monitored IR spectroscopy was reported intending to clarify whether photo-ionization induced isomerization of Ar really occurs or not. IR spectra of the OH stretching vibration clearly demonstrated that the structure in

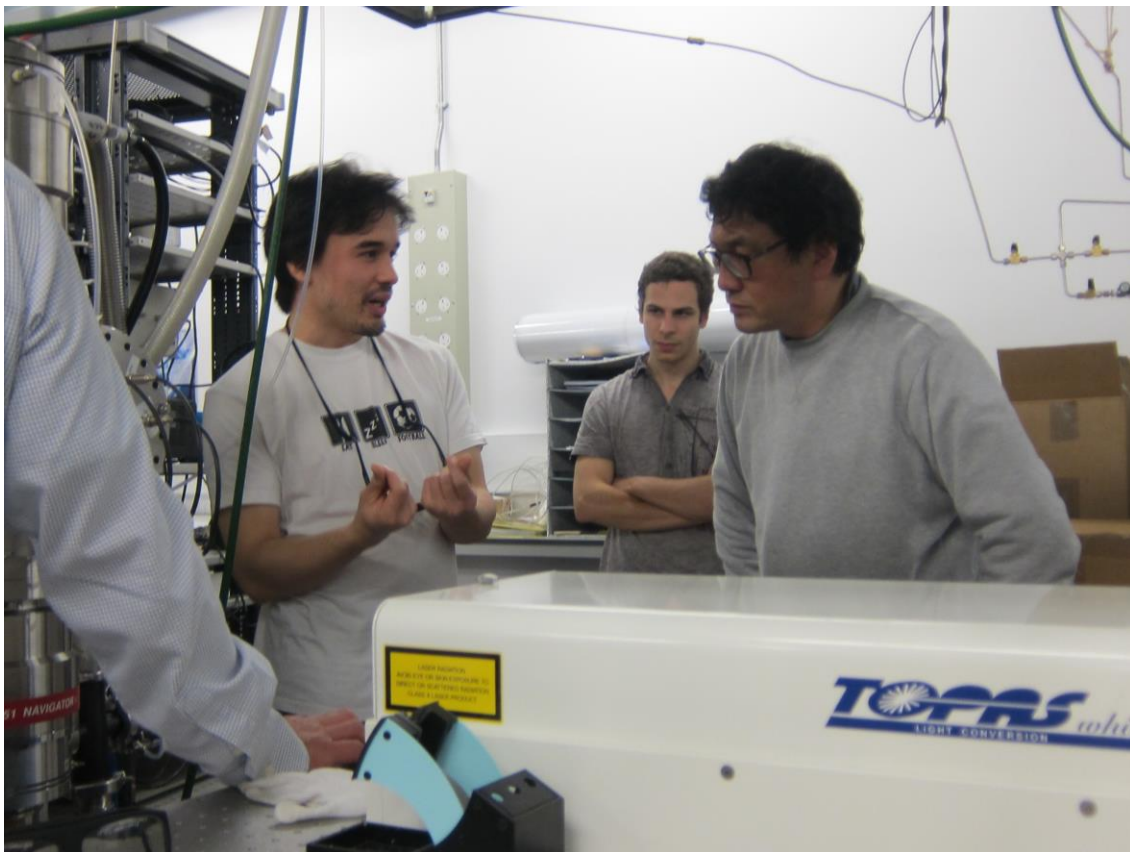
high- n Rydberg states converging IE_0 that is produced by 2-photon ionization from the π -bound structure in the S_0 state keeps the π -bound structure and no sign of H-bound structure was seen. Rydberg states converging to the lowest vibrational level of 15 cm^{-1} energy, on the other hand, shows both the π - and H-bound structures. This result is very important because it would settle the long discussion about the reactivity of $\text{phenol}^+-\text{Ar}$. The next session present a mechanism of water migration and delocalization after photo-ionization of aromatic-diol and -aminoalcohol-water clusters in terms of excess energy and IVR. These results may provide new systems that can be studied by time resolved spectroscopy.

The third session introduced spectroscopy and spectrometry of protonated biologically relevant molecules, such as ubiquitin and amino acids. Further efforts will be aimed at these molecules to trace their dynamics and chemical activity.

After a lunch break, we had two oral sessions for various topics, and a poster session again. Many young graduated students and post-doctoral researchers gave their respective research themes in the sessions. Such a fundamental effort was quite meaningful for us young people to skill up our international scientific communications.



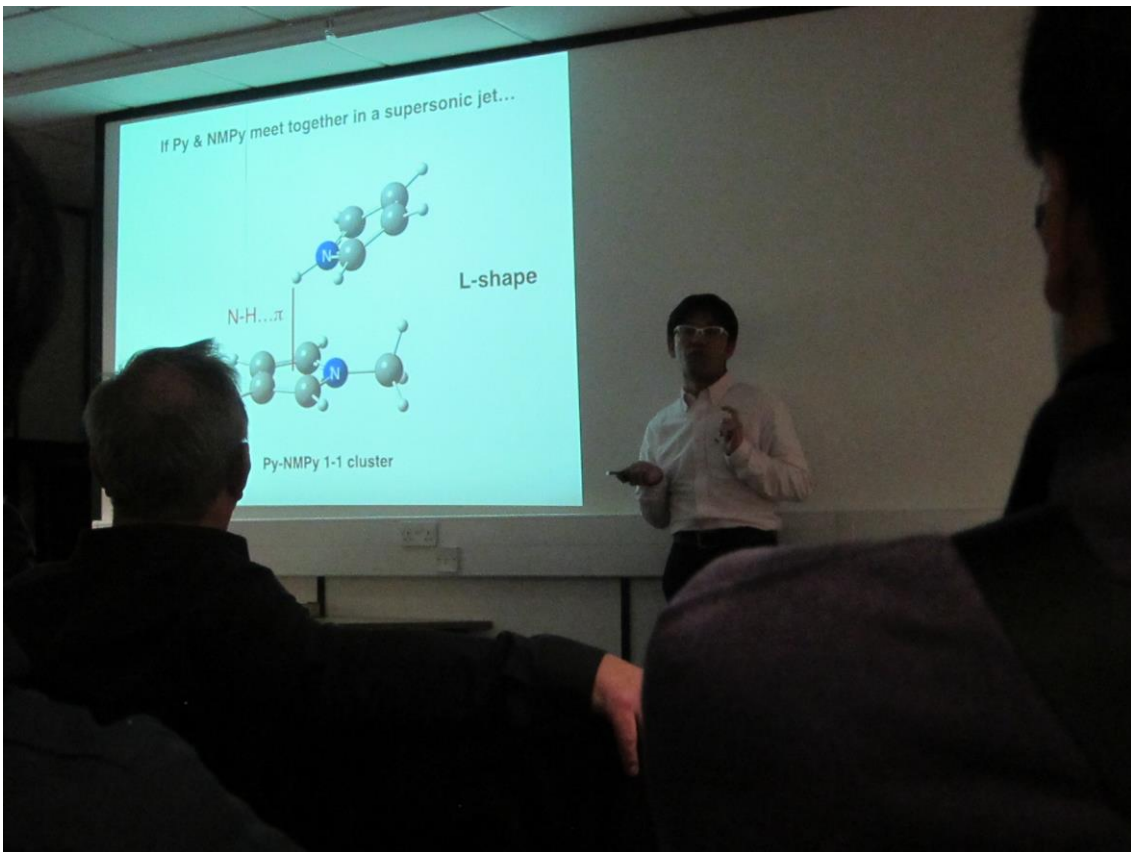
Group photo in Alan Turing Building.



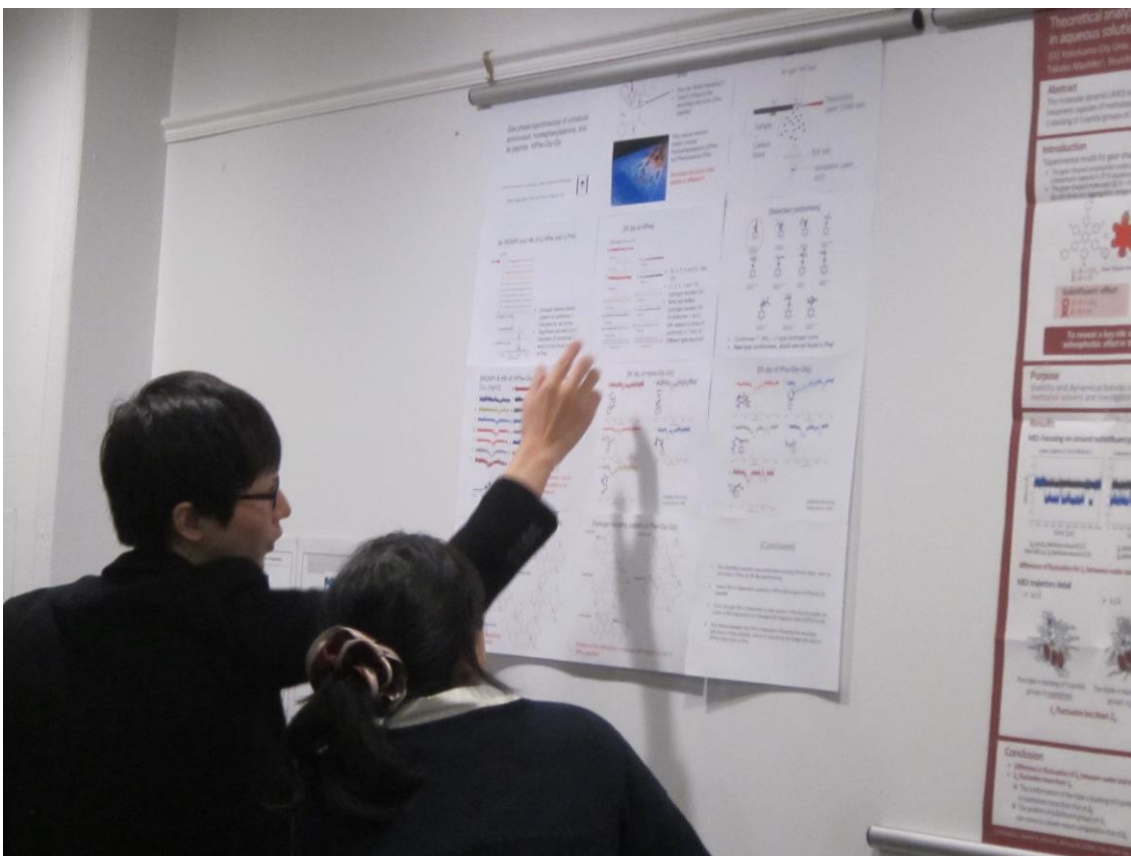
PSI Lab Tour.



Discussion between Prof. Masaaki Fujii and Prof. Maurizio Becucci.



Dr. Yoshiteru Matsumoto, talking about IR Spectroscopy of the Hydrogen-Bonded Clusters.



Discussion in the poster session.