Report of 3rd. Seminar of Core to Core program, "Photoionisation-induced switch in aromatic molecule-solvent recognition", Symposium for Young Scientists

Alan Turing bldg, The University of Manchester, 11th Mar. 2011

Kana Kitatsugu (Tokyo Institute of Technology)

The 3rd. symposium of the Core to Core program was held at University of Manchester on 11th Mar. 2011. The symposium intended to discuss recent progress of intermolecular interaction in aromatic systems and to give a chance for young students to present their research topics in English. The detailed program of the symposium has been shown in another web page (http://www.res.titech.ac.jp/~kiso/CoreToCore/seminar-info-03.html).

The first speaker Prof. O. Dopfer, who is a core member of this project, introduced recent theoretical works on a binding site dependence of the $S_1 \leftarrow S_0$ electronic band origins of phenol-Ar$_n$ (PhOH-Ar$_n$) clusters. Based on the predicted systematic shifts of the origin bands, a new assignment of weak features observed in the REMPI spectra of PhOH-Ar$_n$ was given. The calculations also found local minima that had been missed so far in cationic state of PhOH-Ar$_n$. He proposed a new experimental scheme to elucidate real time dynamics on PhOH-Ar$_2$ cluster by considering the properties of the new assignment and the local minima. The idea is difficult to perform at this stage actually, but has a possibility that opens interesting next step to understand the nature of the interactions.

Next, three master course students, two of which were Japanese and the other was Luxembourg, had presentations. They were asked many questions some of which were not easy for them to answer by professors. Particularly, communications in English is not easy for the Japanese students. We believe, however, such a fundamental effort is necessary especially for Japanese students to skill up their international scientific communications, and is one of the main themes of the Core to Core program.

After that, Dr. M. Kita from Yokohama City University presented theoretical works on electronic states of exotic cations composed of Alkali hydrido and position by sophisticated electronic state calculations. Such a high level treatment of electronic state is also necessary to predict and interpret weak intermolecular interactions that plays central role in aromatic molecule-solvent recognition. The final speaker, Prof. M. Cockett in University of York, talked about another weak intermolecular interaction, NH…π hydrogen bond that is also expected to control biological recognition process. A substituent dependence of the NH…π hydrogen bond strength was discussed based on the IR and electronic spectra of substituted toluene-ammonia clusters. He showed that the interaction site of ammonia drastically changes depending on the substituents inductivity. Such a large change in the binding site is characteristic of weak intermolecular interactions, and the insight of which would be a basis of control of molecular recognition processes. This topic is important because of the close relation to the next extension of the Core to Core program.

Finally, the schedules of the last half of the collaboration were discussed. Plans of travel and experiments at each research center toward the final half year of the program were determined. The symposium is successful as a whole in confirming recent progresses and future of the collaboration.