第 4 回 ICMS 参加および C. Tian 研究室訪問報告

Wang Lin　（東北大・A01 計画班森田グループ）

The 4th International Conference on Molecular Simulation (ICMS) was held at Shanghai on Oct. 23-26. Over the past few decades, molecular simulation has gradually developed into an essential tool which is widely applied in diverse fields including materials science, chemical engineering and biochemistry. This conference provided a platform to exchange ideas, facilitate collaborations, and promote advances to science and technology related to molecular simulation.

Since the 1st ICMS was hosted in Japan in 1994, the number of participants grew with the second and third iterations, in 2004 and 2013. This time, the 4th ICMS was expanded into a major international conference which has over 500 registered participants and more than 200 oral presentations. Although there are many excellent talks, here I only introduce several of them.

The plenary lecture by Prof. William A. Goddard, III (Caltech) introduced the first principles based Reactive force field and the application to complex materials and processes. Prof. Goddard proposed Reactive force field which is based on quantum mechanics (QM) calculations. By using this force field, it is possible to describing reactive processes for millions of atoms and retain QM accuracy. At the same time, he developed the accelerated dynamics for reactive simulations which can extend the time scale to the order of seconds. The methods were successfully applied to oxygen reduction, catalytic conversion and so on.

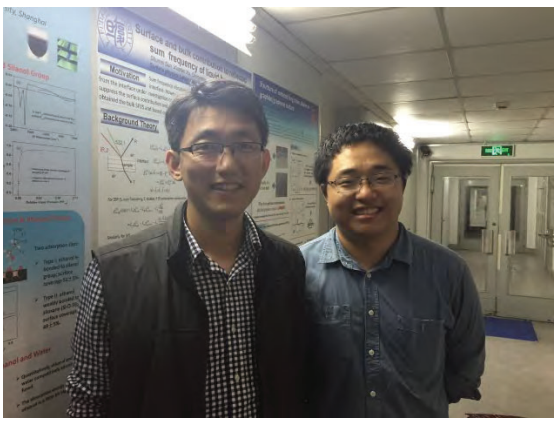
The plenary lecture by Prof. Susumu Okazaki (Nagoya University) introduced the all atom molecular dynamics simulation of polio virus capsids. They developed highly parallelized molecular dynamics (MD) program and used supercomputers to simulate virus up to 10 million atoms. They investigate the stability, response to high pressure, and chemical environment inside the capsid. Further, interaction between the capsid and its receptor has also been studied. The results provide useful information in a molecular level.

The invited talk by Prof. Susan B. Rempe (Sandia National Lab.) introduced the molecular simulation of carbonate solvents for Li^+ electrolytes. They adjusted the force field parameters by fitting the calculated solvation free energy of Li^+ in electrolytes to experimental or QM calculated data. The idea of scaling partial charge is quite instructive.

I also obtained a chance to present my recent work on MD and sum frequency generation (SFG) study of organic electrolyte interface. We developed a general procedure to obtain polarizable and flexible force field for organic compounds and applied it to the simulation of interface structure and SFG. The results provides a detailed understanding of SFG spectra and interface structure of organic carbonates in a molecular level.

This conference provides an excellent platform in molecular simulation field. After communicating with other experts, it is quite helpful for my future study and new research ideas.

On Oct. 27, I was invited to visit Prof. Chuanshan Tian's laboratory in Fudan University. Prof. Tian's research focuses on characterization of material with nonlinear optical spectroscopy. He is an expert on SFG measurement of various interfaces. In the afternoon, after Prof. Morita presented our recent work, I deeply discussed with Prof. Tian and his students about the combination of experimental SFG and molecular simulation study of the interface such as the cation-π interactions in battery system and the possible influence to the interface structure and SFG spectra. This is quite instructive for my future study of solid liquid interface in battery system.



Left: Prof. Tian, Right: Wang Lin @Tian's lab.