

A solution is a complex system, in which a huge number of molecules have a lot of influence on each other. All the molecules continuously change their positions and velocities, which governs chemical reaction in solution phase. While the electronic structure of a molecule is a key to understand the reaction, fluctuations in molecular structure as well as intermolecular interactions are also directly related to the reaction. Therefore a multiscale view becomes important to correctly treat the coupling among these various contributions. In this seminar, I will show the new methods I have developed based on integral equation theory, molecular simulation, and quantum mechanics (QM).