Theory and Computation of Reactions and Properties in Solutions and Liquids

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We focus on the projects both on ultrafast photoinduced electron energy transfer in the excited state in solution and on ionic liquids (ILs). The project on photoinduced electron energy transfer processes in the excited state in solution focuses on the development of a theoretical method to describe electron energy transfer including solvent motion and dynamics. On the other hand, ILs' projects concentrate the study of dynamical properties on ionic liquids with molecular dynamics simulation.

1. The Theoretical Study of Photoinduced Electron Energy Transfer Processes in the Excited State in Solution

We have developed a procedure for tracking the time-dependent evolution of the electronic structure of a solute molecule in solution, coupling an electronic structure theory with solvent motion. We have extended this prescription for studying electron energy transfer processes in the excited state in solution. It is revealed that the coupling between solvation dynamics and a fast intramolecular electron energy transfer is likely to play an important role in the emergence of photo-induced unique functionalities in biochemical and metal complex systems.

2. Investigations of Dynamical Properties on Ionic Liquids[1–2)]

We focus on the dynamical properties on ionic liquids (ILs). With molecular dynamics simulation, it have been found out that ILs indicate unique collective dynamics and distinctive ionic dynamics. We have studied interesting dynamical heterogeneity in ILs at room temperature. Also, we have investigated spatial heterogeneity.

References

1) T. Ishida, The Dynamical Properties on Ionic Liquids: Insights from Molecular Dynamics Study," in *Ionic Liquids—New Aspects for the Future*, J. Kadokawa, Ed., InTech; Rijeka, Croatia, pp. 3–29 (2013).
2) T. Ishida and H. Shirota, *J. Phys. Chem. B* **117**, 1136–1150 (2013).