Theory and Computation of Reactions and Properties in Solutions and Liquids

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We currently 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 is aimed at 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 using molecular dynamics simulation technique.

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

We have developed a procedure for tracing 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 method for investigating electron energy transfer processes in the excited state in solution. It is shown 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, in particular, the dynamical properties on ionic liquids (ILs). With molecular dynamics simulation, it have been found out that ILs indicate unique collective dynamics. We have investigated interesting dynamical heterogeneity in ILs at room temperature. Also, we have studied 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).