

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 is aimed at the development of a theoretical method to investigate electron energy transfer including solvent motion and dynamics. On the other hand, ILs' projects are focused on 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 Solution¹⁾

We have developed a procedure for describing 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 studying 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 Liquids¹⁻²⁾

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

References

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- 2) T. Ishida and H. Shirota, *J. Phys. Chem. B* **117**, 1136–1150 (2013).