Theory and Computation of Reactions and Properties in Solutions and Liquids

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We are interested in 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 study electron energy transfer. On the other hand, ILs' projects are focused on the investigation of dynamical properties on ionic liquids and the unique dissolution process of cellulose polysaccharides using molecular dynamics simulation technique.

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

We have developed a procedure for capturing the time-dependent evolution of the electronic structure of a solute molecule in solution, coupling an electronic structure theory with solvent motion. It is indicated that the coupling between solvation processes and a fast intramolecular electron energy transfer is likely to play an important role in the emergence of photoinduced unique functionalities in biochemical and metal complex systems.

2. Investigations of Ionic Liquids[1–2)] with Molecular Dynamics Simulation

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

References

1) T. Ishida, *AIP Conference Proceedings for 8th International Conference of Computational Methods in Sciences and Engineering(ICCMSE) 2010*, *AIP Conf. Proc.* **1642**, pp. 518–521 (2015).
2) T. Ishida and H. Shirota, *J. Phys. Chem. B* **117**, 1136–1150 (2013).