

Theory and Computation of Reactions and Properties in Solutions and Liquids

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We focus on the projects on ionic liquids (ILs). ILs' projects include both the unique dissolution process of cellulose polysaccharides and the investigation of static and dynamical properties on ionic liquids.

1. Investigations of Dissolution and Decomposition Mechanisms of a Cellulose Fiber in Ionic Liquids¹⁾ with Molecular Dynamics Simulation

We carried out the studies of dissolution and decomposition mechanisms of cellulose (I_β) polymers in ILs. In order to investigate motion of cellulose fibers and intermolecular interactions between cellulose molecules and cationic and anionic species in ILs. We employed the 1-ethyl-3-methylimidazolium acetate IL solvent for target system. From molecular dynamics simulation results, it was found out that the intermolecular interaction energy between cellulose polymers in the IL are reduced, comparing with that in water. Also, our

results suggest that the enhancement of the flexibility of rigid cellulose chains triggered by the breakage of intrachain H-bonds due to anions starts decomposition processes accompanied by dissolution processes due to the intercalation of cations, synergistically, and, then, both dissolution and decomposition processes are executed simultaneously.

2. Researches on Static and Dynamical Properties of Ionic Liquids: Molecular Origin of Low-k Peak of ILs and Dynamical Heterogeneity

We have investigated the molecular level origin of low-k peak ($< 0.5 \text{ \AA}^{-1}$) in the structure factor in ILs. In particular, we found out that the structure factor of heterocyclic ring parts in cations largely contribute to low-k peak in ILs. Also, we are going to carry out the study of dynamical properties of ILs, dynamical heterogeneity in ILs at room temperature with molecular dynamics simulation procedure.

Reference

1) T. Ishida, *J. Phys. Chem. B* **124**, 3090–3102 (2020).