# Theoretical Study of Heterostructures under Light and Voltage Bias

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Heterostructures consisting of different materials have various optical and electronic properties depending on their constituents and the interfacial region. We have studied the heterostructures under light and/or voltage bias using our developed first-principles computational program named SALMON.[1)]

## 1. Photoexcited Electron Transfer in Silver/$TiO_2$ Heterostructure[2)]

The photoexcitation of heterostructures consisting of metallic nanoclusters and a semiconductor causes electron and resonance energy transfers and is extensively investigated to develop photocatalysis and optical devices. Using SALMON, we have studied photoexcited electron dynamics in a silver nanocluster/$TiO_2$ heterostructure. Excited electrons are directly transferred from the silver nanocluster to the $TiO_2$ layer without passing through the silver conduction band because of photoinduced electrostatic interactions at the silver/$TiO_2$ interface.

## 2. Optical Near-Field Excitation of Silicon Semiconductor[3)]

We have clarified that direct interband transitions between different wavenumbers can occur in an indirect band gap semiconductor of silicon by an optical near field (ONF). The energy of the absorption edge can be reduced by the ONF excitation. Furthermore, a large number of transitions are induced by the ONF excitation of the realistic silicon system with a complex band structure more than that of a simplified model system.

### References

1) M. Noda *et al.*, *Comput. Phys. Commun.* **235**, 356–365 (2019).
2) K. Iida and M. Noda, submitted.
3) M. Noda and K. Iida *et al.*, *Phys. Rev. Appl.* **11**, 044053 (7 pages) (2019).

# Theory and Computation of Reactions and Properties in Solutions and Liquids

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We are interested in the projects on ionic liquids (ILs). ILs' projects are focused on the unique dissolution process of cellulose polysaccharides, and the investigation of statical and dynamical properties on ionic liquids including temperature effects.

## 1. Investigations of Dissolution and Decomposition Mechanisms of a Cellulose Fiber in Ionic Liquids[1)] with Molecular Dynamics Simulation

We studied dissolution and decomposition mechanisms of cellulose ($I_\beta$) 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 carried out molecular dynamics simulation. We employed the 1-ethyl-3-methylimidazolium acetate IL solvent for target system. It was found out that the intermolecular interaction energy between cellulose polymers in the IL are reduced, comparing with that in water. Also, it is shown that decomposition and solvation mechanisms of cellulose polymers can be interpreted not only by considering hydrogen bond strength between cellulose chains in the IL, but also by tracking both the intra- and inter-molecular (cellulose) hydrogen bond breaking processes in the IL.

## 2. Researches on Statical 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 ($< 0.5$ Ang.$^{-1}$) 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, to be submitted to *J. Phys. Chem. B*, in preparation.