Electronic Properties of Heterostructures Controlled by Applied Bias and Light

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Heterostructures under applied bias and/or light irradiation have been extensively investigated in relation to the development of optical and electronic devices. To reveal their electronic functions, it is required to clarify the details of the electronic structure under applied bias and the photoinduced electronic interactions at the atomic scale.

1. Optical Response of Heterostructures

We have studied optical response of heterostructures using a first-principles computational program in which electron dynamics is directly calculated in real-time and real-space. This program can be applied to complex optical phenomena such as optical near-field excitation of nanostructures by carrying out massively parallel calculations. Using the program, we have shown that the photoexcitation of a MoS_2-graphene heterostructure induces the electron transfer from graphene to MoS_2. It is revealed that the photoexcitation causes the electron dynamics inherent in atomically-thin interfacial regions.[1)]

2. Electronic Structure Change by Applied Electrode Bias

We have been developing a theoretical approach for describing the electronic structure of heterostructures under applied bias.[2)] It has been shown that change in the electronic properties of heterostructures by an applied bias strongly depends on the atomic scale details of the interfacial region. We further extend the developed approach to address photoexcited systems under an applied bias.

References

1) K. Iida, M. Noda and K. Nobusada, *J. Phys. Chem. C*, in press.
2) K. Iida, M. Noda and K. Nobusada, *J. Chem. Phys.* **146**, 084706 (10 pages) (2017).

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. Also, ILs' projects are focused on the investigation of dynamical properties on ionic liquids including temperature effects 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 investigating the time-dependent evolution of the electronic structure of a solute molecule in solution, coupling an electronic structure theory with solvent motion. It is shown 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 reported that ILs show unique collective dynamics. In addition, we have investigated interesting dynamical heterogeneity in ILs at room temperature. Also, we have studied the solvation mechanism of cellulose polymer in ILs.

References

1) T. Ishida, *AIP Conf. Proc.* **1642**, pp. 518–521 (2015).
2) T. Ishida, in preparation.