

Visiting Professors



Visiting Professor

ASAI, Yoshihiro (from *National Institute of Advanced Industrial Science and Technology*)

Theory of Electron Transport through Single Molecular Bridge Junctions

Theories of transport properties through single molecular bridges and atomic wires between the two electrodes have been investigated.¹⁻³⁾ Special attentions will be paid on heat dissipations accompanying the electron transport. Both fundamental theories and their implementations in terms of first principle electronic structure methods⁴⁾ have been studied, as well as their applications to real non-equilibrium open systems.

Both the physical reality and the chemical reality have been taken into account in the calculations.

References

- 1) Y. Asai and H. Fukuyama, *Phys. Rev. B* **72**, 085431 (2005).
- 2) Y. Asai, *Phys. Rev. Lett.* **93**, 246102 (2004); **94**, 099901(E) (2005).
- 3) Y. Asai and T. Shimazaki, "Vibronic Mechanism for Charge Transport and Migration Through DNA and Single Molecules" in *Charge Migration in DNA, Perspectives from Physics, Chemistry and Biology*, T. Chakraborty Ed., Springer-Verlag; Heidelberg (2007).
- 4) T. Shimazaki and Y. Asai, unpublished.



Visiting Associate Professor

AKIYAMA, Ryo (from *Kyushu University*)

Interaction between Like-Charged Colloidal Particles Immersed in Electrolyte Solution

Study of mesoscopic structure constructed by colloidal particles is important to discuss stability of cytoplasm, formation of rennet gel, and so on. The effective interaction between colloidal particles is necessary to calculate those systems using simulation method, because the molecular simulation with explicit solvent molecule and colloidal particle model is very hard. On the other hand, Kinoshita *et al.* are suggesting the importance of translational motion of solvent molecules to discuss the interaction. Then, we pay attention to the solvent granularity in this study.

We calculate the interaction between like-charged colloidal particles immersed in electrolyte solution using the OZ-HNC theory. Solvent molecules are modeled as neutral hard spheres, and ions and colloidal particles are modeled as charged hard spheres. The Coulomb potentials for ion-ion, ion-colloidal particle, and colloidal particle-colloidal particle pairs are divided by the dielectric constant of water. The van der Waals attraction between the colloidal particles, which is an essential constituent of the DLVO theory, is omitted in our model. Nevertheless, attractive regions appear in the interaction, when the electrolyte concentration is sufficiently high. Then the colloidal particles can adhere each other and can form aggregations or gels in spite of like-charged particles. In our model, the attraction arises from the granularity of solvent molecules. (R. Akiyama, N. Fujino, K. Kaneda, and M. Kinoshita, *Cond. Matt. Phys.* accepted.) We start in to study of Brownian dynamics simulation with the effective interaction and some related chemical reactions.



Visiting Associate Professor

HAYASHI, Michitoshi (from *National Taiwan University*)

Development of a Molecular Theory for Time-Resolved Sum-Frequency Generation and Its Applications to Vibrational Dynamics of Water

We developed a molecular theory for time-resolved sum-frequency generation (SFG). The molecular model for vibrational dynamics of water is constructed using the coupled-oscillator model in the adiabatic approximation. This model allows us to calculate vibrational energy transfer rate constants with two different ways; one is with the dipole-dipole interaction scheme and another is the anharmonicity scheme. An application of this theory is also provided for estimation of the time constants of the intermolecular vibrational energy transfer between water molecules using density functional theory method. This approach can provide a clue of a molecular mechanism as to how vibrational dynamics of water at the surface takes place.