Poster Presentations

P1: 吉田一也（青山学院大理工）

Dynamic response of lipid vesicles to addition of acetonitrile

In this study, we show the dynamics of dioleoylphosphatidylcholine (DOPC) liposomes in response to addition of acetonitrile which is a toxic organic solvent and is widely used in the field of chemistry and industry. It was found that addition of acetonitrile induces the three types of dynamics, which are bursting, deformation, and shrinkage, in DOPC liposomes. We mainly investigated the major bursting dynamics. The percentage of bursting liposomes was reduced with decreasing acetonitrile fraction of additional solution, and we could not find the bursting vesicle in the case of addition of acetonitrile solution with ultra-pure water of 4:6 (vol/vol) and below. The result indicates that acetonitrile with high fraction causes the bursting of liposomes. We also measured elapsed time from the beginning of addition of acetonitrile to beginning of response at each vesicle. The histograms for each fraction of acetonitrile indicate that the elapsed time required for vesicle bursting in the case of low-acetonitrile-fraction solution is longer than that of high fraction. We concluded that the large amount of acetonitrile molecules increase the spontaneous curvature of membranes and induce the vesicle bursting because the invasion speed is higher than flip-flop rate of acetonitrile.

P2: 千葉文野（慶應義塾大学）

Amorphous solids of isotactic poly(4-methyl-1-pentene)

Recently we have found that melted state of isotactic poly(4-methyl-1-pentene) shows a pressure-induced structural change. In this study we made amorphous solids of the same polymer. One amorphous solid is made by quenching its melted state at atmospheric pressure. Another amorphous solid is made by press working. The x-ray diffraction patterns of these two solids show differences in their structures.

P3: 池田晴國（名古屋大学理）

The correlation length of the glass transition

A liquid cooled under its melting temperature is called supercooled liquid. With decrease of the temperature, the relaxation time of supercooled liquids shows dramatic increase, and eventually overcomes the observation time. This phenomenon known as the glass transition is widely observed when liquids are quenched so fast as to avoid crystallization.

One of the most significant features of the glass transition is that although the relaxation time of supercooled liquids increase over a dozen orders of magnitude, the configurations of molecules look just as random as that of liquids. In the case of thermodynamic phase transitions, the relaxation time grows with the static correlation length, i.e. the origin of the slow dynamics is the collective motion of a macroscopic set of particles. Though it is plausible that there is the hidden collective motion behind the glass transition, to detect this is difficult because the configuration of glasses looks as random as liquids.

In this study, we tried to estimate the correlation length from the behavior of confined supercooled liquids. We perform the calculation for high dimensional model liquids, and succeed to determine the critical exponent of the correlation length under the mean-field approximation.

P4: 勝部翔太郎（島根大学教育）

Self-assembly organogels composed of 2-naphthaol + AOT organogels in nonpolar solvents

Shotaro Katsube, Tatsuya Umecky, Toshiyuki Takamuku, Yukiteru Katsumoto, Toshihiko Kaji, Masahiro Hiramoto, and Katsura Nishiyama

We have synthesized organogels composed of a surfactant, AOT, and 2-naphthol in nonpolar solvents by self-assembly. We have found that the high transparency of the 2-naphthol gel up to 98% is suitable for optical materials. In addition, the 2-naphthol gel can be applied to light emitting materials, because the framework itself of the gel emit under UV excitation. In this work, we present the results of the 2-naphthol gel surface structures by means of AFM. We also discuss structural, optical and thermal properties of the gels, by using NMR, FTIR, steady-state absorption and emission, and drop-point measurements.

P5: 西山桂（島根大学教育）

Generation of amplified spontaneous emission from Eu complexes dispersed in organogels

Katsura Nishiyama, Yasuhiro Watanabe, Takashi Harada, Kenji Kamada, and Hideki Kawai

The rare-earth complex Eu(hfa)(phen) is dispersed in the organogel composed of p-chlorophenol and a surfactant, AOT, which is gelled in nonpolar solvents by self-assembly. The time profiles of the emission intensity observed from the complex-organogel system suggest the possible generation of amplified spontaneous emission. From a viewpoint of the host material, the organogel can support eight times as much of the complex with better emission quantum yield. A theoretical estimation of the laser gain factor of the complex-organogel also proposes that this system might have application in laser systems.

P6: 宮田竜彦（愛媛大学理工）

Accuracy of Solvation Free Energy Estimated from Hypernetted Chain and Kovalenko-Hirata Approximations for Two-Component Lennard-Jones Liquid

The accuracy of both hypernetted chain (HNC) and Kovalenko-Hirata (KH) closures assumed in an Ornstein-Zernike integral equation theory has been studied in terms of the solvation free energy (SFE) by comparing with molecular dynamics simulation for Lennard-Jones liquid. The Lennard-Jones parameters for the solute were systematically varied. While epsilon_u-dependence of the relative SFE is hardly dependent on the approximations, sigma_u-dependences of the SFE obtained both from HNC and KH approximations considerably differ from those by molecular dynamics simulation. The source of the error in the SFE from both approximations is also discussed.

P7: 井上雅郎 （九州大学理）

Application of the Time-Dependent Density Functional Theory to Microrheology

We study microrheology of a colloidal dispersion system by the time-dependent density functional theory (TDDFT). We consider a hard-sphere probe particle embedded into a colloidal dispersion system. The probe particle is pulled at a constant velocity. Then, the probe particle is subjected to the resistance force due to the collision with colloidal particles. Our purpose is to clarify effects of interactions between colloidal particles on the resistance force.

The resistance force is determined by the concentration distribution of colloidal particles around the probe particle. We numerically calculate the concentration distribution using TDDFT. This theory has been successful in describing the dynamics of simple liquids and colloidal dispersion systems. Also, in the present study, we ignore hydrodynamic interactions due to a solvent.

The calculated results show that the resistance force decreases because of hard-sphere interactions between colloidal particles for slow velocities. A significant effect of the interactions is caused by the increase in the volume fraction of colloidal particles. Also, the effect of the interactions is more significant for small colloidal particles than for large particles. In contrast, for fast velocities and large volume fractions, the resistance force increases because of hard-sphere interactions between colloidal particles.

P8: 川畑雄一 （九州大学理）

Preferential Interaction in Hard-Sphere Mixture System: Integral Equation Study

The crowders' effects on the stability of a protein are often discussed in the viewpoint of the preferential interaction. If the excluded volume effect based on repulsive interactions is dominant in the system, it is expected that the chemical potential of a protein decreases due to the preferential solvation of large crowders. To evaluate this effect quantitatively, we studied the chemical potential in hard-sphere mixture systems which have no attractive interaction.

We solved the HNC-OZ equation for the system which contains solvent (small-sized sphere), crowders (medium-sized sphere), and a solute (large-sized sphere), varying the composition of the mixture at constant pressure. To calculate the chemical potential of the solute, we adopted two methods; one was based on Morita-Hiroike equation, and the other was Kirkwood-Buff theory.

We obtained opposite tendencies for two methods when the size of the crowder molecule was large. In the case of Morita-Hiroike equation, the chemical potential increased with increasing the concentration of crowders, while it decreased in the case of Kirkwood-Buff theory. This disagreement indicates that investigation of the HNC approximation's validity is needed.

P9: 澤山 拓斗（九州大学理）

Assembly of acidic proteins and attractive patches mediated by multivalent cations

Assembly of proteins is important in biological function. For example, an actin filament is assembly of G-actin and is necessary for construction of cytoskeleton and amoeboid movement. Structural studies suggest that multivalent cations are important as mediators of the assembly of acidic proteins.

We calculated an effective interaction between macroanions immersed in electrolyte solution using an integral equation theory. The results indicate that the strong attraction between macroanions appears only when the cation-concentration is medium. To discuss the effective attraction between acidic proteins with the attractive patches which are carboxylate oxygens, we calculate an effective interaction between oxygen sized ions. The results show that assembly of oxygen sized ions occurs by mediation of only multivalent cations not monovalent. We also discuss the assembly of proteins with taking account of an influence of electronic potential of macroanions.

P10: 中村有花（九州大学理）

Effects of solvation structure on diffusion and breakdown of the Stokes-Einstein relation

To study the effects of the solvation structure on the diffusion of a solute particle, we calculate the diffusion coefficient for a variety of solute sizes. For the calculation, we employ a perturbation theory developed by us recently. In this theory, the solvation structure is considered through the radial distribution function between solvent and solute particles. The calculation results of hard sphere system show the breakdown of the Stokes-Einstein (SE) relation even when the solute particle is 10 times as large as the solvent particle. Additionally, the deviation from the SE relation increases with the packing fraction of solvent spheres. This deviation is caused by the solvation effect since the solvation structure is not considered in the SE relation.

P11: 山下拓海 （九州大学理）

Solvent Effects on Protein-Protein Interaction in an Electrolyte Solution: A Study Based on Charged Hard Sphere Model

The effective protein-protein interaction w(r) = -kTln[g(r)] is obtained from the Fourier transfer of the structure factor S(k) given by small angle scattering experiment. Here g(r) is radial distribution function. Basically, w(r) has been discussed on the basis of S(k) with a continuous solvent model. However, Kinoshita et al. have been discussed remarkable effects arising from the translational motion of solvent molecules. We studied the solvent effect on S(k) under weak coupling conditions to discuss the validity of conventional picture.

We calculated w(r) using an integral equation theory. We examined two models: Charged hard spheres with explicit solvent (Model_1) and with implicit solvent (Model_2). Although the g(r) for the Model_2 did not indicate any significant peak at the contact distance of proteins, the g(r) for the Model_1 did. It was arising from the translational motion of solvent molecules. In spite of this difference in g(r), these structure factors S(k) were nearly the same each other. This result suggests that the solvent effects should be lost in the analysis and the continuous solvent model has been justified. We may report the w(r) which is simulated by MC using effective potential energy between two particles Veff2(r) calculated in infinite dilution model.

P12: 山田一雄 （九州大学理）

A unified proof of the Harada-Sasa equality for underdamped and overdamped Langevin systems

We derive a new expression for the violation of the fluctuation-response relation (FRR) in the colloidal dispersion systems by multiple-time scale analysis. The new expression unifies the Harada-Sasa equality both in the underdamped and overdamped Langevin models. The Harada-Sasa equality connects the magnitude of the FRR violation with the rate of the stationary energy dissipation. We also elucidate that the Harada-Sasa equality is valid in a new time region, which differs from that in the underdamped and overdamped model. The perturbative expression is obtained by the expansion of the violation of FRR in powers of $\varepsilon = m/\gamma$, where γ is the friction coefficient and m is the mass of the particle. The Harada-Sasa equality is valid up to the second order of ε when time t satisfies $\varepsilon \ll t \ll \gamma f/L$. Here, f is the stationary driving force, and L is the characteristic length of the system, respectively. In addition, we derive the expression in the fluctuating hydrodynamic model, where the fundamental quantities are given by the density and momentum fields of the colloidal particles. We represent the Harada-Sasa equality by these field variables.

A reference-modified density-functional theory for improving solvation free energy

Recently, Miyata clearly showed a theoretical drawback of the hypernetted-chain (HNC) approximation for solvation free energy (SFE) of solutes in the case of Lennerd-Jones (LJ) fluid [1]. Similar theoretical drawback has been pointed out in the case of hydration free energy of various solute molecules in water: the hydration free energy monotonically increases as the size of solute molecules increases. In the study presented here, we propose a reference-modified density-functional theory (RMDFT) for improving the theoretical drawback of the HNC approximation. In this approach, we employ a hard-sphere fluid as a reference system of the DFT instead of an ideal gas that is a standard reference system of classical DFT for simple liquids. The RMDFT provides correction terms for the HNC approximation not only on SFE but also on radial distribution functions. We applied the RMDFT to bulk and infinitely diluted solutions of LJ systems. The result of solute-size-dependence for SFE obtained from the RMDFT agrees well with the molecular simulation result reported by Miyata [1]. The RMDFT approach would have a high possibility on the theoretical improvement of the liquid state theory for molecular fluids.
[1] T. Miyata and J. Thapa, Chem. Phys. Lett. 604, 122 (2014).

Emergence of a new ice phase in the course of crystallization to ice VII

We report various types of pathways emerging in the course of freezing into a high pressure ice VII by large-scale molecular dynamics simulations at 10 GPa, 425 K. Some trajectories showed an apparently stepwise transition via the unique metastable "phase" in accordance with Ostwald's step rule. The metastable structure was identified as one of the tetrahedrally close-packed structures having the nature of a rotator phase (plastic phase). The unit cell consists of 21 water molecules that has not yet been reported by simulation or by experiments. On the other hand, once the embryo of ice VII appears prior to that of the metastable phase in liquid, direct transition to ice VII takes place. We also show that the plastic (rotator) behavior of the metastable phase is not uniform but is sensitive to the interaction strength of adjacent molecules and the local structure.

P15: 阿部紀遥（岡山大学自然）

Mean field analysis on the local solubility of nonpolar molecules in the liquid-vapor interface of water

Solubility of nonpolar gases both in bulk water and in the interfacial water has been extensively studied. Recently, we found that the local solubility of Lennard-Jones (LJ) methane at the liquid-vapor interface of water decreases with increasing temperature when the solvent density around the solute molecule is fixed. The next step is to clarify what properties in the solvent structure are responsible for the monotonic decrease in solubility.

Here we present a mean field approach on the methane/water interfacial system, replacing the solute-solvent LJ interaction potential with the hard-sphere plus the LJ attractive tail. With the test particle theory, we decomposed the solubility into two contributions: the probability of cavity formation and a conditional average of a Boltzmann factor associated with the solute-solvent attractive interaction energy.

The temperature variation of two quantities is obtained by molecular dynamics simulation. We confirmed that this mean field approximation does not change the qualitative behavior of local solubility obtained from the full LJ potential. For any fixed local solvent density, we found that the probability of cavity formation is almost invariant with temperature while the average of the Boltzmann factor decreases with temperature.

[1] Kenichiro Koga, *Phys. Chem. Chem. Phys.*, 13, 19749 (2011).

P16: 村上達哉（岡山大学自然）

Phase transition between plastic crystal and crystal in the square-well dumbbell model

A plastic crystal is a solid material in which molecules are oriented in a random way while their centers of mass are arranged in order. Recently a computer simulation study has shown strong evidence for an existence of a critical point between a high-pressure ice (ice VII) and the corresponding plastic ice [1]. Although there are many other plastic crystals such as those of polymers, nitrogen, oxygen, and C60, so far existence of other critical points has not been reported or possibility of the existence has not been explored in a systematic way.

The purpose of the present study is to find fundamental conditions for the existence of the critical point associated with a plastic crystal. One of the simplest is a hard-dumbbell model whose phase diagram is well known [2]. The calculated phase diagram for this purely repulsive-interaction model, however, does not have a critical point. Thus we study the hard-dumbbell model with an attractive square-well potential. From the NPT ensemble Monte Carlo simulations, the phase boundary between crystalline and plastic solid phases is determined in the temperature-pressure plane. With these results, we will discuss possibility of the critical point for this model.

[1] K.Himoto, M.Matsumoto and H.Tanaka, *Phys. Chem. Chem. Phys.*, 16,5081 (2014)
[2] C.Vega, E.P.A.Paras and P.A.Monson, *J. Chem. Phys.*, 97, 8543 (1992)

P17: 山本伸也（福岡工業大学）

Liquid crystal phases of layered perovskite nanosheets with varied layer thickness

A series of liquid crystalline colloids of the inorganic nanosheets with varied layer thickness of 1.2- 2.4 nm were prepared by exfoliation of Dion-Jacobson-type layered perovskites, $KCa_2Na_{3-n}Nb_nO_{3n+1}$ (n = 3, 4, 5, and 6), and their isotropic/liquid crystal phase transition behavior and structure were investigated. The birefringent textures observed by polarized microscopy confirmed the formation LC phase in the colloid. Swollen lamellar structures were identified by small-angle X-ray scattering, while the basal spacing increased to up to 144 nm with increase in n. The colloids with large basal spacing showed weak greenish or bluish structural colors.

P18: 原諒平（九州大学理）

A theoretical method of calculating a solvent dynamical effect on a solute insertion into a cylindrical vessel

The static effect of solvents on a biological process has often been studied. However, the dynamical effect of solvents does not clear. Our purpose is to develop the theoretical method of studying the dynamic effect of solvents on a biological process. For the purpose, we use the time dependent density functional theory. In the theory, the microscopic interaction between solvents is included.
 The theory is applied to the insertion process of a solute into a cylindrical vessel immersed in solvents. Solvents and a solute are hard-sphere models. The vessel is hard-core model. We calculate the non-equilibrium spatial distribution of solvent number density in the case that a solute is in inserted into the vessel with a constant velocity. As a result, the distribution of the solvent deviates from the equilibrium distribution of the solvent.