The 5th Mini-Symposium on Liquids (MSL2011)
List of Poster Presentations
June 25, 2011

Pre-Poster Session (12:00~12:55)
Poster Preview Session and Poster Presentations (14:45~17:00)

P1: K. Abe, and K. Koga (Okayama University)
Phase transition in a quasi-one-dimensional lattice

Abstract:

We investigate phase behavior of liquids confined to nano pores, using a nearest-neighbor lattice model. The model is characterized by two parameters which represent different substances, and also by the width of the lattice. The phase behavior of our model is obtained from MC simulation. Other results for the case where the nearest neighbor interaction is not isotropic are also given.

P2: Y. Kubota, and R. Akiyama (Kyushu University)
Triplet Distribution Functions for Hard Spheres Calculated by Monte Carlo Simulation and Integral Equation Theories.

Abstract:

Nowadays, three-dimensional integral equation theories become important methods to study protein folding, molecular recognition, self-assembly phenomena and other various phenomena in condensed phase. The information given by those methods has multi-body correlation. It, then, is much more fruitful than the information given by the Kirkwood superposition approximation. The difference between the simulation's results and the superposition approximation's results becomes large, when ligand-binding phenomena by a narrow concave recognition site are examined. We can find the test of the three-body correlation for the Born-Green-Yvon 2 theory when the packing fraction is 0.275. However, the test of the HNC approximation for water's packing fraction (0.38) is important because of biological interest. Here, we compare the triplet distribution functions given by 3D-HNC-OZ theory with those given by the superposition approximation and given by the Monte Carlo Simulation. The agreements are qualitatively and semi-quantitatively good. We will compare between the results given by some approximations.

P3: H. Akiyoshi, and K. Koga (Okayama University)
Diffusion coefficient of argon in single walled carbon nanotubes

Abstract:

Diffusion coefficient of argon in single walled carbon nanotubes (SWNT) depends on not only temperature, pressure (density) also tube diameter. In this study, we conducted isochoric-isothermal molecular dynamics simulation to understand relationship between pore size and diffusion coefficient at same temperature and pressure. Previous study proved that diffusion coefficient depends on simulation cell size on the bulk fluids. Therefore, we examine whether argon in SWNT depends on simulation cell size or not. Moreover, computational study have shown that argon in SWNT have many structures depended on temperature, pressure and pore size. Thus, this study suggests the relationship between diffusion coefficient and those structures, and between diffusion coefficient and density.

P4: Y. Aoyanagi, and K. Okumura (National Institute of Advanced Industrial Science and Technology (AIST))

Simple Model for Mechanics of Spider Webs

Abstract:

The spider web is mainly composed of two types of threads. One is radial thread. Another one is spiral thread. It’s well known that the radial threads make the frame work of web and the radial threads are stiff. The spiral thread has viscoelastic property and very soft. Here, we have a question. Why are the radial threads stronger than the spiral threads? We propose a simple model to describe spider orb webs [1]. The model has a formal analytical solution when no thread elements are broken. When the radial threads are sufficiently strong compared to the spiral threads, the model is free of stress concentrations even when a few spiral threads are broken. This is in contrast with what occurs in common elastic materials. According to our model, spiders can increase the number of spiral threads to make a dense web (to catch small insects) or adjust the number of radial threads (to adapt to environmental conditions or reduce the cost of making the web) without reducing the damage tolerance of the web.

[1] Yuko AOYANAGI and Ko OKUMURA, A simple model for the mechanics of spider webs, Phys. Rev. Lett. 104, 038102 (2010); featured in, Philip Ball, Web designers, Nature Materials 9, 190 (2010).

P5: T. Araki, and A. Onuki (Kyoto University)

Behaviors of charged particles near a water-oil interface

Abstract:

In a phase-separated binary solvent, a charged particle prefers to be immersed in a more polar liquid like water. This is because the electrostatic energy is reduced when the particle is in a more polar phase. In addition, the surface of a charged particle is usually hydrophilic. Our numerical and theoretical studies reveal that the wetting behavior of charged particle can be controlled by adding hydrophobic salt into the binary solvent. In particular, the particle can be trapped at the interface of the demixed solvent, in an intermediate range of the concentration of the hydrophobic salt. We also argue a possible application of charged colloids to a Pickering emulsion, in which the electrostatic interaction among the particles lying at the interfaces may change the interface property.

P6: A. Eri, and K. Okumura (Ochanomizu University)

Dynamics of drops and bubbles in a Hele-Shaw cell

Abstract:

We have studied the dynamics of liquid drops and air bubbles in a quasi two-dimensional confined space (i.e., in a Hele-Shaw cell). In this symposium, we discuss about the lifetime of bubbles [1], viscous drag friction acting on fluid drops [2], and bursting of a thin film [3] in a Hele-Shaw cell. Our experimental results can be explained by original and simple scaling arguments.

[1] A. Eri and K. Okumura, Lifetime of a two-dimensional air bubble, Phys. Rev. E 76, 060601(R) (2007).
[2] A. Eri and K. Okumura, Viscous drag friction acting on a fluid drop confined in between two plates, Soft Matter, in press.
[3] A. Eri and K. Okumura, Bursting of a thin film in a confined geometry: Rimless and constant-velocity dewetting, Phys. Rev. E 82, 030601(R) (2010).

P7: L. Hakim, M. Matsumoto, K. Koga, and H. Tanaka (Okayama University)

Phase behavior of gas hydrate of cubic ice and ice II structure

Abstract:

The occupancy of hydrogen inside the voids of cubic ice and ice II, which gives two stable hydrogen hydrate compounds at high pressure and temperature, has been examined using a hybrid grand-canonical Monte Carlo simulation in wide ranges of pressure and temperature. The simulation reproduces the maximum hydrogen-to-water molar ratio and gives a detailed description on the hydrogen influence toward the stability of ice structures. A simple theoretical model, which reproduces the simulation results, provides a global phase diagram of two-component system in which the phase transitions between various phases can be predicted as a function of pressure, temperature, and chemical composition. A relevant thermodynamic potential and statistical-mechanical ensemble to describe the filled-ice compounds are discussed, from which one can derive two important properties of hydrogen hydrate compounds: the isothermal compressibility and the quantification of thermodynamic stability in term of the chemical potential.

P8: Y. Hamamoto, and K. Okumura (Ochanomizu University)

Analytical Studies on a Crack in Simplified Nacre Model

Abstract:

Nacre is composed of thin layers of soft protein and hard CaCO3 platelets. Although the soft protein occupies only 5 volume % of the composites, it is known that this layered structure shows remarkable strength compared with a hard monolithic CaCO3. One possible mechanism was proposed through a simple model and an exact solution for the model [1]. Here, we develop the derivation in a heuristic way [2] and provide a new analytical

solution by which we can discuss more familiar situation in the fracture mechanics [3]: the previous solution was limited to the stress distributions around a semi-infinite crack but the present new result reveals that around a finite crack. Furthermore, we discuss analytical solutions for multi-cracks.

[1] Ko Okumura and Pierre-Gilles de Gennes, Eur. Phys. J. E 4 (2001) 121.
[2] Yukari Hamamoto and Ko Okumura, J. Eng. Mech. 135 (2009) 461.
[3] Yukari Hamamoto and Ko Okumura, Phys. Rev. E 78 (2008) 026118.

P9: S. Hayaki, K. Kikui, K. Kido, D. Yokogawa, H. Sato, and S. Sakaki (Kyoto University)

An Application of RISM Method Incorporating Intramolecular Fluctuation

Abstract:

Room-temperature ionic liquids (ILs), which consist of bulky cations and anions, have drawn enormous interest because of their intriguing features such as exceptionally high CO2 storage capacity. In this work, we utilized RISM method incorporating intramolecular fluctuation to investigate the ratio of isomers of 1-butyl-3-methyl-imidazolium halogen ([bmim][X]: X = Cl, Br, or I) and dissolution structure of CO2 in [bmim][PF6]. The obtained intramolecular correlation functions of [bmim][X] suggested that the ILs composed of smaller halogen anions, which generates stronger electrostatic field, tend to be densely packed to form gauche conformer. The calculated pair correlation functions showed that the Coulomb interaction between CO2 and [PF6]- plays an important role in the dissolution of CO2.

P10: K. Himoto, M. Matsumoto and H. Tanaka (Okayama University)

Structure and connectivity of plastic ice

Abstract:

We have investigated structural and energetic characteristics of plastic ice, which was found in high pressure region such as 10 GPa by molecular dynamics simulation and free energy calculation. It was predicted that plastic ice intervenes between ice VII and liquid water, in which diffusion is suppressed but rotation is allowed. In the present work, structure in plastic ice is explored from both local and global view points and focus is placed on the local arrangement, the extent of deviation from the ideal lattice position, and the hydrogen-bonded patterns. The roles of the attractive interaction and the repulsive part of Lennard-Jones potential are also examined. It is found that the higher interaction energy in plastic ice induces a large dislocation of water molecules, which eventually conducts a facile rotation. There are large amount of hydrogen-bonds which do not orient to the tetrahedral directions. These orientational defects give rise to fusion of the two interpenetrating sublattices of ice VII leading to plastic phase rather than defect-containing ice VII, which results in unique network structure of the plastic ice.

P11: M. Hishida, and K. Tanaka (Kyoto University)

Long-range hydration effect of lipid membrane studied by terahertz time-domain spectroscopy

Abstract:

The hydration state of biomolecules is believed to affect their self-assembly. In the present study, the hydration state of phospholipid bilayers is observed precisely by terahertz spectroscopy, by which water perturbed by a lipid membrane is detected sensitively from the observation of the relaxation dynamics of water molecules in the subpicosecond time scale. Combined with x-ray observation of the lamellar structure of the lipid, a long-range hydration effect on up to 4-5 layers of water (1nm thickness) is confirmed. Most water molecules in the lamellae fall into the hydration water, and condensation of them is also indicated.

P12: T. Kaneko, T. Akimoto, K.Yasuoka, A. Mitsutake, and X. C. Zeng (Keio University)

Dynamical coexistence and size dependence of water cluster

Abstract:

Water clusters exist in interstellar or high altitude air, but the cluster size effect on physical properties is not completely understood. In this study, Multicanonical and canonical molecular dynamics simulation of water clusters are performed and dynamical coexistence and size dependence are studied.

P13: Y. Kawashima, T. Sakata, S. Yamamoto, H. Nakano, K. Nishiyama, and R. Akiyama (Kyushu University)

Solvent effect of the absorption and fluorescence spectra

Abstract:

Molecular dynamics simulation based on Quantum Mechanics / Molecular Mechanics method are performed to construct absorption and fluorescence spectra of coumarin 120 in water. The solvent effect on the absorption and fluorescence spectra is analyzed by decomposing it into two contributions: one from the motion of the solute molecule, and the other from the polarization of the solvent molecules.

P14: K. Koga (Okayama University)

A general view on solvation of apolar solutes in water and in simple liquids

Abstract:

Solvation of apolar solutes in a model water and that in simple liquids are compared and contrasted. Qualitative similarities are found for the solvation processes in fixed-volume conditions whereas significant differences manifest themselves when the constant-pressure solvation processes are assumed. Solvation thermodynamics is presented in a way that includes solvation processes with an arbitrary, microscopic volume change and relates the solvation thermodynamic quantities to appropriate temperature derivatives of the excess chemical potential.

P15: Y. Kubota, and R. Akiyama (Kyushu University)

Model Dependence of Dielectric Response to Molecular-Sized Ion in Water

Abstract:

The dielectric response of water governed by solute molecules has been studied using various methods because it is an important topic in the study of electron transfer reactions and of the hydration energy of a solute. We have examined water polarization phenomena caused by a solute charge using molecular dynamics (MD) simulations. When the solute charge is small, the polarizability of the water varies remarkably and the maximum value of the polarizability is twice that for a neutral solute. And it began to decrease, when the peak position was exceeded. With increasing the absolute value of the solute charge, the response to the solute charge was not saturated, and it approached a linear response behavior. Our results showed not only a strong nonlinearity of the dielectric response but also fine structure in the polarizability curve. It seems that the structure is caused by the microscopic change of solvation structure, for example breaking of hydrogen-bond network. However, there is a possibility that the fine structure depends on the water model. Then, we examine the fine structure for various models of the water.

P16: M. Matsuo, Y. Takii, M. Matsumoto, and H. Tanaka (Okayama University)

Thermodynamic Stability of CO_2 clathrate hydrates

Abstract:

Clathrate hydrates are nonstoichiometric compounds in which guest molecules are contained in the lattice made of water molecules. All the water molecules are tetrahedrally coordinated in a similar way as ice at low pressure but it is made of polyhedra in which guest molecules are encapsulated. Two sorts of crystalline form with a single guest species at low pressure are known as structure I and structure II. Carbon dioxide forms structure I clathrate hydrate but its occupancy in smaller cage is controversial. In this study, we examine whether the smaller cages contain carbon dioxide molecules by Grand-canonical/NPT Monte Carlo simulations [1] at 270 K. It is found that the occupancy for the smaller cage increases to 0.4 at 200 MPa while it is negligibly small at low pressure such as 3 MPa.

[1] K.Katsumasa, K. Koga and H. Tanaka, J. Chem. Phys. **127**,044509 (2007)

P17: T. Miyata (Ehime University)

Brownian Dynamics Simulation of Self-Diffusion of Ionic Large Solute Molecule in Modeled Polyelectrolyte Gel

Abstract:

We study the self-diffusion of ionic large solute molecule in a model of polyelectrolyte gel by Brownian dynamics simulations. In particular, we examine the relationship between the self-diffusion coefficient and the

parameters describing the structure of polyelectrolyte gels. In the time-dependence of the mean square displacements, three time-scales are observed. The self-diffusion coefficient is evaluated from the time-dependence of the mean square displacement in the long time-scale. A couple of structural parameters of gels are tested to correlate them with the self-diffusion coefficient. Furthermore, a simple theoretical formula for the self-diffusion coefficient is proposed based on the Smoluchowski equation.

P18: H. Mizuno, and R. Yamamoto (Kyoto University)

Rheological behaviors of a supercooled liquid under general shear strains

Abstract:

Simple liquids usually behave as Newtonian fluids under shear flows. However, even simple liqiuds, when cooled to supercooled state, show non-Newtonian behaviors, whose origin still remain elusive. The past reaserches have invesitgated the rheological behaviors of supercooled liquids in a simple situation, where a steady shear flow is applied in one direction. On the other hand, in the case of complex fluids such as polymer solutions, their rheological behaviors have been invesitgated under more general shear strains such as oscillatory shear strain or two shear strains at the same time. So, in this study, we investigated the rheological behaviors of a supercooled liquid under general shear strains. We considered the constitutive equation in the tensor form, which can describe well the rheological behaviors of a supercooled liquid.

P19: T. Murashima, and T. Taniguchi (Kyoto University)

Advection of Microscopic States in Entangled Polymer Melt Flow

Abstract:

In general, macroscopic flow involves positional displacements not only at the macroscopic level but also at the microscopic level because of its microscopic dynamics. Because such positional displacements at the microscopic level do not affect macroscopic flow behavior in many cases, we can ignore to treat the microscopic dynamics when we solve the macroscopic flow. However, in polymer melt flow, the positional displacements, namely the change in polymer conformations, markedly affect its flow behavior because of its anisotropic structure. Especially in entangled polymer melt, the correlation between entangled polymers is history-dependent because of their topological constraint. Therefore, advection mechanism for microscopic states in the macroscopic fluid dynamics have to be managed in an appropriate manner which depends on the focused dynamics at the microscopic level. We overview advection mechanisms of microscopic states through polymer melt flow simulations, and then we conclude that the Eulerian description for the macroscopic flow requires some statistical treatment that loses the microscopic details; the Eulerian description is not appropriate for the entangled polymer melt flow with the molecular pictures.

P20: Y. Nakamura, A. Yoshimori, and R. Akiyama (Kyushu University)

A perturbation theory for friction of a large particle immersed in a binary solvent

Abstract:

We have developed a new theory of a binary solvent to study effects of a distribution of circumjacent solvent particles on friction. Here, we consider the friction from solvent particles to a large solute particle, such as a protein, moving in a binary solvent. To develop the theory, we employed perturbation expansions by assuming that a solvent particle was much smaller than a solute particle. From the expansion, an analytical expression of the friction was obtained, including the radial distribution functions of a binary solvent. Using our theory, we calculated the friction of a hard-sphere system, varying the size ratio and packing fraction.

P21: K. Nishiyama, N. Yoshida, and F. Hirata (Shimane University)

Solvent Effects on Fluorescence Spectra of Coumarin 153. A comparative study of RISM-SCF Calculations and Spectroscopy

Abstract:

We have applied RISM-SCF theory to describe electronic structures of a dye molecule, coumarin 153, in the ground and excited states, immersed in solvents with various polarity and chemical structures. We compare the theoretical results with the steady-state fluorescence Stokes-shift measurements.

P22: N. Obara, and K. Okumura (Ochanomizu University)

Universal scaling law for the imbibition of textured surfaces with ”soft” edges

Abstract:

Micropatterned surfaces have been studied extensively for a number practical effects of wetting [1, 2] or hydrodynamics [3]. Dynamics of the imbibition of porous or textured surfaces has been quantitatively studied since the classic paper by Washburn in 1921 [4]. Recently, thanks to the modern photolithographic technique, surfaces with more regular texture formed by a forest of cylindrical pillars of micron scale have become available. The dependence of Washburn dynamics on texture geometry (i.e., pillar height, distance, and radius) is established as simple power laws in two different regimes at long and short times. In this case of long pillars with sharp edges the film thickness propagating on the surface is virtually the same as the pillar height [5, 6]. Here, we study the ”opposite” case where the texture on surfaces are composed of shorter pillars of ”soft” (or non-sharp) edges. As a result, we find a universal scaling law, different from the Washburn law and independent of texture geometry, and the film thickness not equal to the pillar height.

[1] Quéré D (2002) Surface chemistry: Fakir droplets. Nature Materials 1:14–15.

[2] Tuteja A, et al. (2007) Designing superoleophobic surfaces. Science 318:1618–1622.

[3] Cottin-Bizonne C, Barrat JL, Bocquet L, Charlaix E (2003) Low-friction flows of liquid at nanopatterned interfaces. Nature Materials 2:237–240.

[4] Washburn E (1921) The dynamics of capillary flow. Phys. Rev. 17:273–283.
[5] Ishino C, Reyssat M, Reyssat E, Okumura K, Quéré D (2007) Wicking within forests of micropillars. Europhysics Letters 79:56005–1–56005–5.
[6] Hamamoto-Kurosaki M, Okumura K (2009) On a moving liquid film and its instability on textured surfaces. European Physical Journal E 30:283–290.

P23: R. Sakamaki, A. Sum, T. Narumi, and K. Yasuoka (Keio University)

Phase equilibria for common water models

Abstract:

Vapor/liquid and liquid/solid (proton-disordered hexagonal ice phase) phase equilibria for common water models were studied by using molecular dynamics simulations. The direct coexistence method used in this work is known to require larger amount of computational power than other methods including the free energy method or Gibbs ensemble, but be accurate. The interfacial tension and coexistence density, pressure and temperature for common water models will be presented in our poster, and the best (or better) water model for vapor/liquid and liquid/solid phase equilibria will be discussed.

P24: T. Sekiguchi, M. Tani, and K. Okumura (Ochanomizu University)

Experimental study on the Brazil nut effect

Abstract:

We report on an experimental study of the Brazil nut effect. For this purpose, we observed the ascent of a large disk imbedded in a two-dimensional packing of small beads vertically vibrated. We examined the rising speed of the large disk, and identified a constant velocity part. We found an interesting sharp dependence on acceleration of the rising velocity.

P25: T. Sumi, and H. Sekino (Toyohashi University of Technology)

How the liquid-liquid transition affects hydrophobic hydration of a polymer chain in supercooled water

Abstract:

A density-functional theory (DFT)-based multiscale simulation of a hydrophobic polymer chain in supercooled water is presented. The DF model for water reproduces hydrophobic collapse of the polymer chain at room temperature and low pressure and also demonstrates pressure-induced unfolding even at room temperature. The result indicates that the DF model can reproduce water-like solvation thermodynamics at room temperature. As the temperature decreases less than the liquid-liquid critical point, we observe a significant swelling at low-density liquid (LDL) phase but no specific change at high-density liquid (HDL) phase. The polymer behavior is qualitatively agreed with that in the Jagla fluid. Our result strongly suggests the qualitative similarity

of solvation thermodynamics between water and the Jagla fluid near the liquid-liquid phase transition.

P26: N. Takahashi, and K. Okumura (Ochanomizu University)

On the stress concentration in a simple elastic-plastic model

Abstract:

When there is a line crack in an elastic plate, the stress is enhanced at the crack tip. This phenomenon is called stress concentration and is one of the principal factors governing the strength of material. This phenomenon played a key role, when one of the authors created a simple simulation model for a spider web and showed that the combination of soft spiral thread and hard radial thread is important for the strength [1]. In this study, we investigate the stress concentration in a two dimensional elastic-plastic network. As a result, we numerically find simple scaling relations between the crack-tip stress concentration and the mesh size. This result indicates that materials can be strengthened, thanks to large voids.

[1] Yuko AOYANAGI and Ko OKUMURA, A simple model for the mechanics of spider webs, Phys. Rev. Lett. 104, 038102 (2010). PDF inside only; featured in, Philip Ball, Web designers, Nature Materials 9, 190 (2010).

P27: Y. Takehara, and K. Okumura (Ochanomizu University)

High-velocity drag friction in dense granular media

Abstract:

We measured directly the drag friction in a high-velocity region (a few 100 mm/s) and confirmed an original scaling law [1]. For the theoretical interpretation, we made a nontrivial assumption on behavior peculiar to granular media and developed an original theory. We conclude that the observed friction is physically different from a hydrodynamic inertial friction, which has been discussed in previous works. We further discuss the relation of the present work to the jamming transition.

[1] Y. Takehara, S. Fujimoto and K. Okumura, High-velocity drag friction in dense granular media, EPL 92, 44003 (2010).

P28: M. Tani, T. Sekiguchi and K. Okumura (Ochanomizu University)

Imbibition of inhomogeneous textured surfaces

Abstract:

Dynamics of the penetration of liquid into textured surfaces follows a simple power law similar to that of the classic theory of capillary rise. Recently, this dynamics for textured surfaces was shown to be characterized by parameters of the texture geometry (pillar height, distance, and radius) in two different regimes [1,2]. We briefly

review the previous studies and explain our recent attempts to make inhomogeneous textured surfaces using a modern photolithographic technique. Furthermore, we discuss novel imbibition dynamics emerging from inhomogeneous textured surfaces and our current trials of experimental confirmation of the dynamics.

[1] Chieko Ishino, Mathilde Reyssat, Etienne Reyssat, Ko Okumura, David Quéré (2007) Wicking within forests of micropillars. Europhysics Letters 79:56005-1--5.
[2] Minako Hamamoto-Kurosaki, Ko Okumura (2009) On a moving liquid film and its instability on textured surfaces. European Physical Journal E 30: 283–290.

P29: R. Tatsumi, and R. Yamamoto (Kyoto University)

Numerical Simulation Analysis of Ultrasound Attenuation in a Colloidal Solution

Abstract:

We developed a direct numerical simulation method for colloidal dispersions with a compressible solvent fluid. With this method, attenuation of ultrasound propagating through a colloidal solution was investigated quantitatively.

P30: R. Teshigawara, and A. Onuki (Kyoto University)

Pre-dewetting transition on hydrophobic substrate: statics and dynamics

Abstract:

We investigate phase transitions of van der Waals fluids on a hydrophobic substrate. When we put a liquid on a hydrophobic substrate, a vapor layer appears on the substrate. Its thickness can change discontinuously as a first-order phase transition, depending on the temperature and the bulk density of the liquid, which is called "pre-dewetting transition". We will also present dynamic behaviors around this transition after a change of the boundary temperature.

P31: K. Tokunaga, T. Furumi, and R. Akiyama（Kogakuin University）

A Model Study of Energy Conversion from Chemical Reaction into Mechanical Work through Solvation

Abstract:

The intermolecular interactions are usually changed due to a chemical reaction. Mechanical work is often produced from the interaction changes. Beginning of the energy conversion is hydrolysis of ATP in case of ATP-binding protein (e.g. actin-myosin motor protein system). If we regard the reactant as a solute, the other molecules are regarded as a solvent environment. In this study, we examine a possibility of conversion from chemical reaction into mechanical work due to solvation change around the reaction site. A simple model is adopted as the system and the molecular dynamics (MD) simulations are carried out with the explicit solvent

model. Motion of the motor protein, energy conversion mechanism, and dependence of the motion on the solvent density will be discussed in the poster session.

P32: T. Yamaguchi, and S. Koda (Nagoya University)

Molar conductivity minimum of electrolyte solutions in solvents of low polarity

Abstract:

The molar conductivity of electrolyte solutions often shows a minimum as the function of concentration when the dielectric constant of the solvent is low. The mechanism is analyzed with molecular simulation, theoretical calculation, and experiments. It is revealed that the conventional static association models do not apply to the molar conductivity minimum, and collective dynamics of ions should be taken into account.

P33: Y. Yamakawa, M. Matsumoto and H. Tanaka (Okayama University)

Structure and dynamics of aqueous solutions of electrolytes in confined space

Abstract:

We have investigated aqueous solutions of electrolytes in nanotube to explore microscopic picture of transport process of hydrated ions (potassium chloride) in confined space. Because of the small number of ions in the system, structural and dynamic properties suffer from large fluctuations. In order to affirm convergences of those properties, molecular dynamics simulations are carried out in which all the possible initial arrangements of ions are examined. Convergence is slow but an equilibrium ion arrangements is attained after reasonable simulation time. Gradual exchange of ions leads finally to the alternate arrangement of cation and anion in most of the cases. In the poster session, we show time evolution of ion-arrangement and discuss a relation between structure and potential energy of ions.

P34: M. Yokota, and K. Okumura (Ochanomizu University)

Dimensional crossover in the coalescence dynamics of viscous drops confined in between two plates

Abstract:

We investigated the coalescence of viscous drops in a Hele-Shaw cell [1]. Here, we report two original scaling laws which appear at short times and long times in a single coalescence event. We clearly show that the transition of the dynamics from the short-time regime to the long-time regime is brought about by a crossover from a three-dimensional viscous dynamics for a spherical drop to a quasi two-dimensional one for a disk drop. In addition, we discuss an unusual type of coalescence that is possibly caused by naturally accumulated electric charge in the confined geometry and whose dynamics seems self-similar.

[1] Maria YOKOTA and Ko OKUMURA, Proc. Nat. Acad. Sci. (USA), 108 (2011) 6395; featured in In this issue (This week in PNAS), PNAS, 108 (2011) 6337.

P35: T. Yoshidome, Y. Ito, M. Ikeguchi and M. Kinoshita (Kyoto University)

Importance of water entropy in rotation mechanism of F1-ATPase

Abstract:

We propose a novel picture of the rotation mechanism of F1-ATPase, a rotary-motor protein complex [1]. Entropy, which originates from the translational displacement of water molecules, is treated as the key factor in the proposal [2]. We calculate the hydration entropies of three different sub-complexes comprising the gamma subunit, one of the beta subunits, and two alpha subunits adjacent to them. The calculation is performed by a hybrid of the angle-dependent integral equation theory [3] and the morphometric approach [4]. The major finding is that the packing in F1-ATPase is highly asymmetrical and this asymmetry is ascribed to the water-entropy effect. We discuss how the rotation of the gamma subunit is induced by such chemical processes as the ATP binding, ATP hydrolysis, and release of the products. In our picture, the asymmetrical packing plays crucially important roles and the smooth rotation is driven by the water-entropy effect.

[1] T. Yoshidome, Y. Ito, M. Ikeguchi, and M. Kinoshita, J. Am. Chem. Soc. 133, 4030 (2011).
[2] M. Kinoshita, Front. Biosci. 14, 3419 (2009).
[3] M. Kinoshita, J. Chem. Phys. 128, 024507 (2008).
[4] R. Roth, Y. Harano, and M. Kinoshita, Phys. Rev. Lett. 97, 078101 (2006).

P36: A. Suematsu, A.Yoshimori, M.Saiki, J.Matsui, T.Odagaki (Kyushu University)

Application of a phase transition theory to a glass forming system

Abstract:

We have shown why a system does not crystalize but forms glass using the density functional theory with a thermodynamic perturbation method. We apply the theory to the Lennard-Jones-Gauss(LJG) system. It is shown that the LJG system does not crystalize by molecular dynamics simulations. Using this theory, we decide whether a solid or a liquid phase is more stable, at a wide range of parameters. In addition, we show that the system does not crystalize because of high transition density of a solid.

P37: Y. Yoshitake, and K. Okumura (Tokyo Denki University)

Effect of Surface Structures on Contact Angle Hysteresis

Abstract:

We study contact angle hysteresis on textured surface when the volume of a two-dimensional liquid drop is increased or decreased. The surface energy of the drop has a periodic form governed by the surface pattern. The contact lines are trapped at local minima of surface energy. This causes pinning and depinning of the contact lines with the volume change. We show that the CAH emerges from this simple scenario even though we do not take any effect of viscous dissipation into account.