lipid molecules and/or hydrogen-bond making and breaking dynamics with water molecules. Therefore, terahertz time-domain spectroscopy (THz-TDS) is a powerful tool to investigate lipid molecule dynamics. In this study, we focus on dependence of the low-frequency dynamics of lipid bilayers on hydration, temperature, and their structure by using THz-TDS. As a sample, we selected 1, 2-Dimyristoyl-*sn*-glycero-3-phosphoglycerol (DMPG), which is known to form several different structures like crystalline or gel phase states. We measured the temperature dependence of the low-frequency spectra of the DMPG under different hydration degrees and structures. The absorption coefficients of each sample were obtained in the frequency region from 10 cm⁻¹ to 50 cm⁻¹. We discuss about the dynamics of DMPG from the changes of the absorption coefficients.

3PT157 表面張力レプリカ交換法による脂質二重膜の構造サンプリング

Surface tension replica exchange molecular dynamics method for an efficient sampling of lipid bilayer structures

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Generalized ensemble algorithm is one of the efficient sampling methods for biomolecular systems. Recently, various replica exchange molecular dynamics methods (REMD) in different parameter spaces have been developed. However, simulations for membranes or protein-membrane systems are still difficult with generalized ensemble algorithms, because the membrane can easily collapse in such enhanced sampling methods like temperature REMD. To overcome this problem, we propose a new replica exchange molecular dynamics method, where the surface tension of the system in an NPyT ensemble is exchanged (γ REMD). Exchanging the surface tension can moderately induce the deformation of lipid bilayers. We introduced γ REMD in our laboratory-developed MD program (GENESIS), and it was applied to a fully hydrated 1,2-di-palmitoyl-phosphatidylcholine (DPPC) lipid bilayers. We found that the area per lipid and membrane thickness can change significantly in the γ REMD simulation, compared to the single NPyT simulation. We believe that our method is useful for investigating structural properties of lipid bilayers, conformational changes of membrane proteins in membranes, and protein-lipid interactions.

3PT158 膜厚変化とゲル、アミノ酸、水素化アモルファスシリコンを用いたイオン伝導整流素子の特性

Film thickness and property of ion conductive rectification element using amino acids, gel and hydrogenated amorphous silicon

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This report mainly focuses an electro-potential-current property correlated with film thickness on ion conductive rectification element using amino acids, gel and hydrogenated amorphous silicon. In general, ionic conduction, in solution as well as in intermediate states between a liquid and a solid, such as gels, is a phenomenon key to inter-conversion between light energy, chemical energy, and electric energy. As such, this phenomenon is essential for devices that store, generate, and convert electric energy, including batteries, photovoltaics, capacitors, and actuators. This report secondly focuses on ionic conduction in nontoxic materials to discuss the creation of elements coated with multi-layer functional thin-films using a combination of different technologies, such as the rectification property of ionic conduction, photo-induction control, and the use of wavelength conversion materials, and the potential application of these materials to biological tissue. Ion conductive behaviors of neutral, acidic, or basic amino acid dispersed in agarose gel are characterized. We report an attempt of measuring a photo-controlled effect of a-Si:H film on ion conducting behavior of bio-molecules in detail, comparing several thickness of a-Si:H film.

3PT159 BLM を介したイオン性蛍光プローブの膜透過性—電流と蛍光に基づいた動的解析—

Permeability of an ionic fluorescent probe through a BLM - dynamic analysis based on an electric current and a fluorescent change-

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Transport of an ionic species through a bilayer lipid membrane, BLM, is influenced not only by its hydrophobicity but also by a coexisted counter ion, and the transport mechanism has been considered to be complicated. Recently, new opinion for the BLM transport of an ion has been reported by Shirai et al. [1, 2]. In the opinion, a BLM was recognized as like a thin liquid membrane with two aqueous/membrane interfaces. The transferring ion distributes to a BLM with coexisted counter ion and transports across the BLM keeping electroneutrality in the BLM. Electrochemical results were given as experimental evidences for the transport mechanism, but not enough for supporting the cotransport mechanism which is not detected by electrochemical measurement. In the present work, an ionic fluorescent probe was employed as the transferring ion through a BLM. Transport of the probe was detected not only as the ion transfer current but also as fluorescent change near to the BLM induced by the ion transport. Comparing the transport current with the fluorescent change, whether the transferring species is ionic or neutral was estimated. According to the observation, the mechanism of ion transport through a BLM was discussed. [1] O. Shirai, S. Kihara, Y. Yoshida, M. Matsui: J. Electroanal. Chem., 389, 61-70 (1995) [2] O. Shirai, Y. Yoshida, M. Matsui, K. Maeda, S. Kihara: Bull. Chem. Soc. Jpn., 69, 3151-3162 (1996)

3PT160 ABC トランスポーターのヌクレオチド結合ドメインに対する ATP 結合自由エネルギー計算

Calculation of the binding free energy of ATP to the nucleotide binding domain of an ABC transporter

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ABC (ATP-binding Cassette) transporters exist in almost all kinds of living things and use ATP as an energy source to transport a wide range of substrates across the membrane. ABC transporters have the common 3D structural architecture: the whole molecule is divided into two domains, that is, Transmembrane Domain (TMD) and Nucleotide-Binding Domain (NBD). NBD has two highly conserved ATP binding sites (Walker A&B and LAGGQ). It has been proposed that binding of ATPs to these sites induces the dimerization of two NBDs, eventually leading to a large structural change from the inward- to outward-facing conformation of TMD.

Our study is to elucidate this structural change mechanism from energetic aspects. In this study, as a first step, we evaluated the free energy gain obtained from binding of the ATP to NBD. We examined this for NBDs in the maltose transporter (MalFGK₂) from *Escherichia coli*. For this purpose, molecular dynamics (MD) simulations were performed starting from the crystal structure of the NBD dimer and subsequently the above free energy was calculated according to the MM/PBSA method.

We first evaluated the binding energy of one ATP molecule to an NBD monomer. The resultant values were -37.6 and 4.1 kcal/mol when ATP binds to the Walker A&B motif or the LSGGQ one, respectively. Next, the NBD dimerization energy was evaluated to be -5.91 kcal/mol. We are now calculating the binding free energies of ADP and inorganic phosphate (Pi) to an NBD to elucidate the role of ATP hydrolysis in the substrate transportation process.

3PT161 パターン化モデル生体膜へのロドプシンの再構成

Reconstitution of rhodopsin into micropatterned model biological membrane

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Rhodopsin (Rh) is a photoreceptor that forms a complex with transducin (G_t) upon activation by light. It has been reported that the affinity of Rh*-G_t complex to lipid rafts (raftophilicity) was higher than that of Rh (Hayashi et al. ARVO meeting (2011)). We are developing a methodology to evaluate the raftophilicity quantitatively with a supported phospholipid bilayer (SPB). Micropatterned SPBs composed of photo-polymerized lipid bilayer and fluid lipid bilayer. By changing the compositions of polymeric and fluid bilayers, liquid ordered (l_o) domains and liquid disordered (l_d) domains in the fluid bilayer were separated into a pre-determined pattern. To measure the localization of Rh and Rh*-G_t in l_o regions, we incorporated Rh into SPB by rapid dilution of Rh/ octylglucoside micelles. We confirmed single Rh molecules in SPB by TIRF-microscopy. Furthermore, we observed binding of fluorescently labeled α -subunit of G_t (G_{at}) upon activation of Rh and changes in