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Hydration water dynamics between DMPE (1,2-dimyristoyl-sn-glycero-3-phosphoethanolamine) phospholipid bilayers by quasi-elastic neutron scattering

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Terahertz time domain spectroscopy (THz-TDS) revealed that fast (rotational) water dynamics depend on phospholipid headgroup structure by comparing PC and PE [1], but the comparison between them for the loosely and tightly bound (translational) hydration water (HW) observed for DMPC by quasi-elastic neutron scattering (QENS) [2], is still not revealed. We have done QENS experiments on the d54-DMPE+10D2O, to observe DMPE headgroup modes. After separating the headgroup modes, we analyzed the QENS profiles of HW from the d54-DMPE+10H2O by the sum of three Lorentz functions corresponding to slow, middle speed, and fast modes. The relaxation time of the fast mode is approximately six times faster than that in DMPC estimated by THz-TDS [3]. The diffusion coefficient of the middle speed mode was the same order of magnitude as the free water, the slow mode was approximately the same as that of the loosely bound water observed in DMPC [2], while the tightly bound water was not identified because it may be embedded in the headgroup dynamics. We also found that activation energy estimated from the temperature dependence of the mean residence time of the free water in the vicinity of DMPE is significantly lower than that of DMPC [2]. We will discuss the headgroup dynamics with Molecular Dynamics simulation results.
References: [1] Hishida et al., J. Phys. Soc. Jpn. 2014, 83, 044801. [2] Yamada et al., J. Phys. Chem. B 2017, 121, 8322. [3] Choi et al., J. Chem. Phys. 2012, 137, 175101.

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