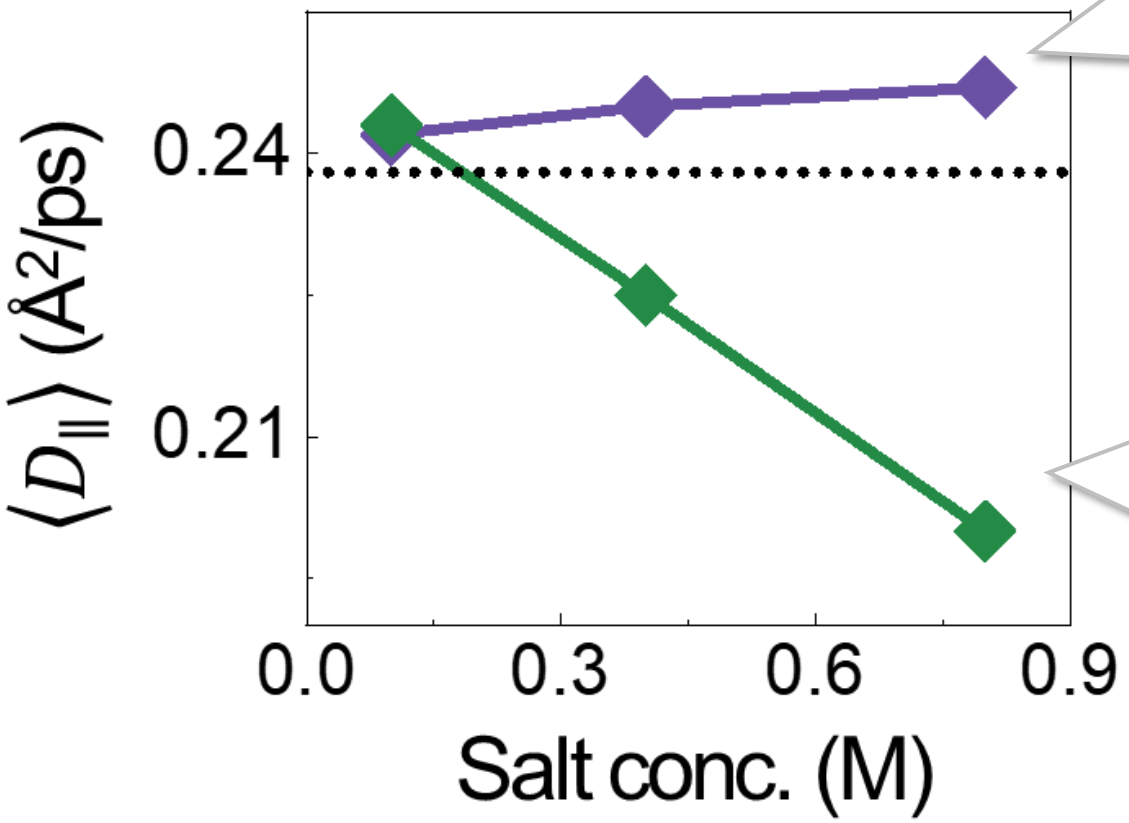
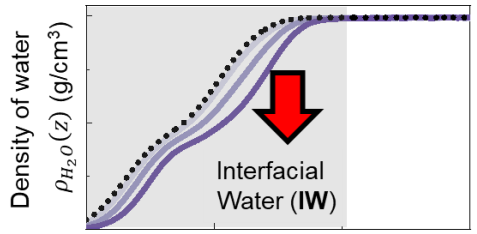
SI Result 1. Mean Diffusion Coefficient

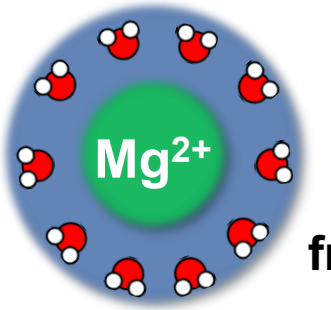
$$\langle D_{\parallel} \rangle = \lim_{t \to \infty} \frac{\Delta_{2,\parallel}(t)}{t}$$



Fraction of IW decreases. (See **Result (3)**)



$$\langle D_{\parallel} \rangle = D_{\parallel,\mathrm{IW}} \cdot f_{\mathrm{IW}} + D_{\parallel,\mathrm{B}} \cdot f_{\mathrm{B}}$$



$$D_{\parallel}^{\mathrm{H_2O\cdots Mg^{2+}}} \ll D_{\parallel}^{\mathrm{H_2O}}$$

As Mg^{2+} Conc. Increases, fraction of bound water increases.

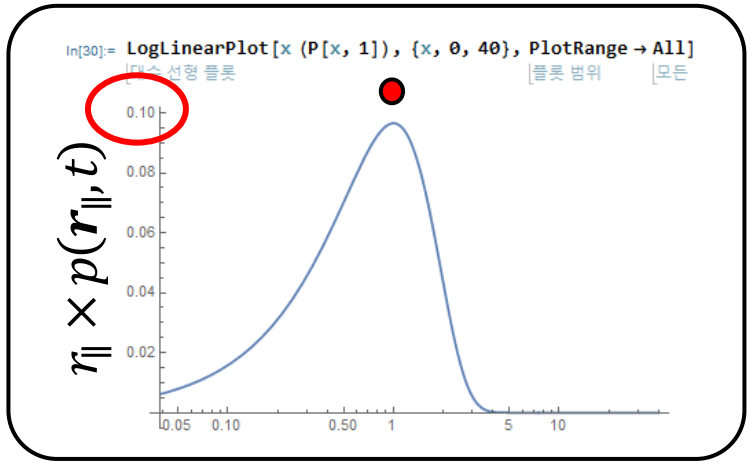
SI Result 2. Lateral Displacement Distribution

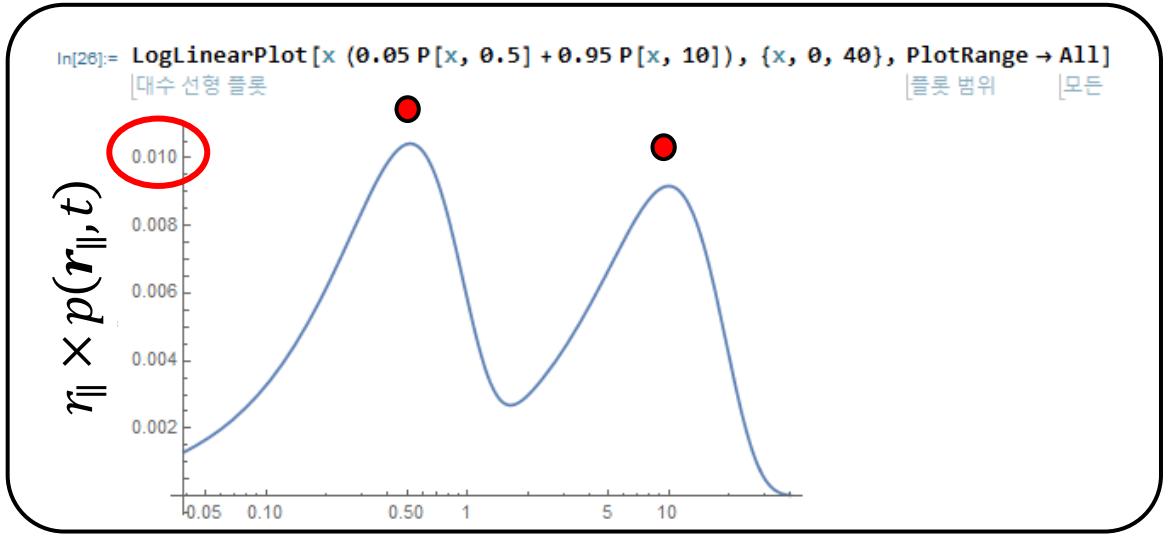
$$p(\boldsymbol{r}_{\parallel}, t) \cong \sum_n f_n p_{\mathcal{N}}\left(\boldsymbol{r}_{\parallel}, t | D_{\parallel}^{(n)}\right) \qquad \sum_n f_n = 1$$

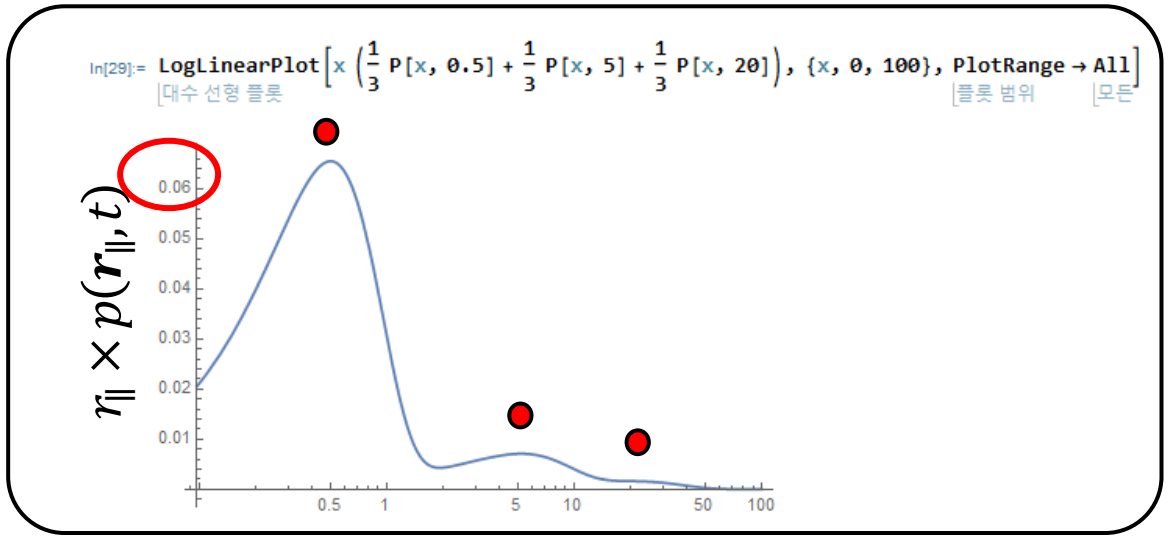
$$p_{\mathcal{N}}(\boldsymbol{r}_{\parallel}, t | D_{\parallel}) \equiv (4\pi D_{\parallel} t)^{-1} e^{-r_{\parallel}^2 / 4 D_{\parallel} t}$$

$$r_{\parallel} \times p_{\mathcal{N}}(\boldsymbol{r}_{\parallel}, t | D_{\parallel}) \rightarrow \text{maximum at } r_{\parallel} = \sigma = \sqrt{2 D_{\parallel} t}$$

```
In[2]:= P[x_, σ_] := (2 π σ²)^-1 Exp[-x² / (2 σ²)]
                     지수 함수
```





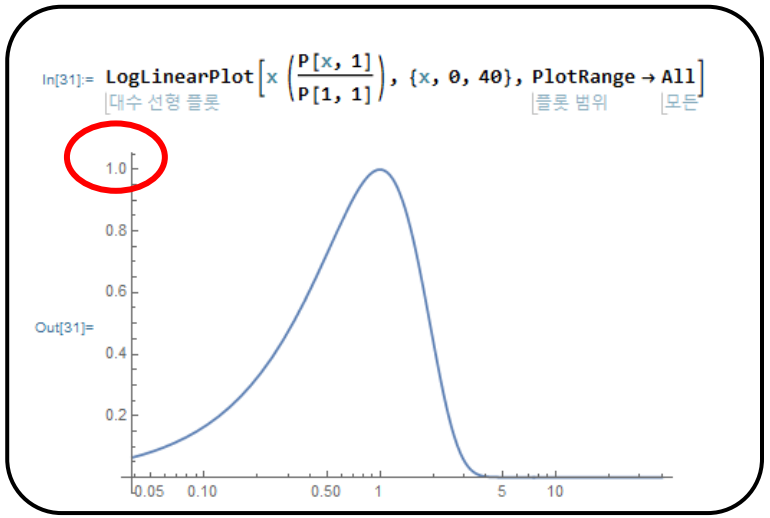


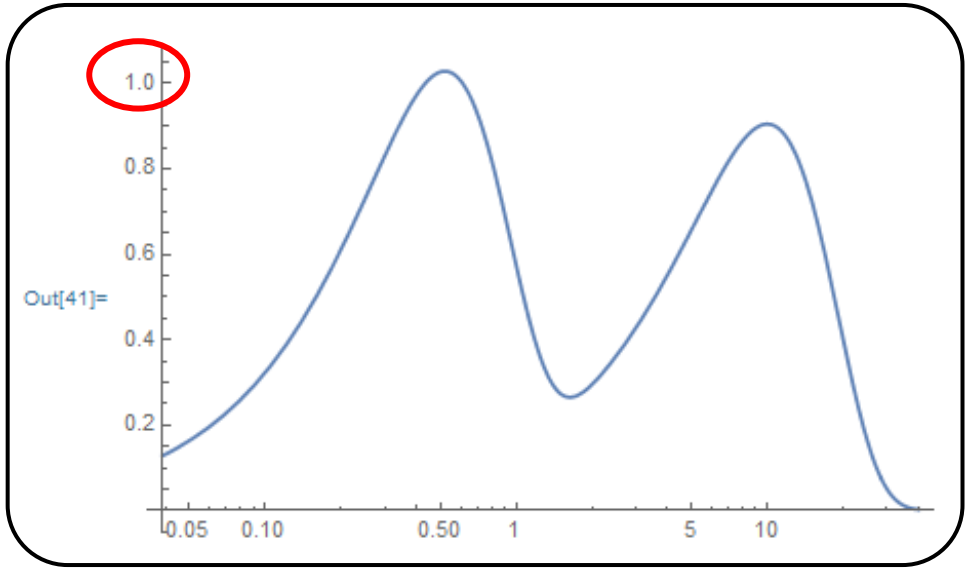
SI Result 2. Lateral Displacement Distribution

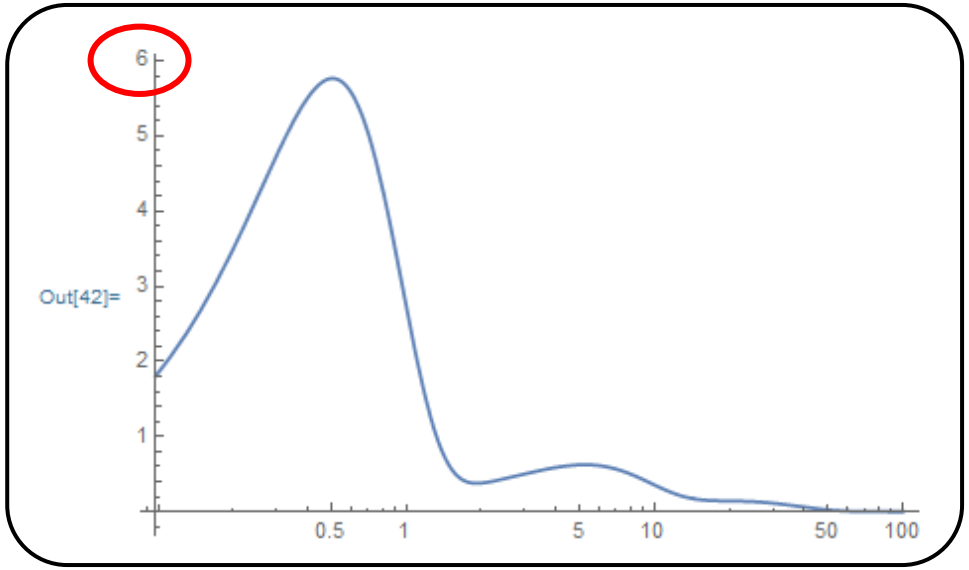
$$p(\boldsymbol{r}_{\parallel},t) \cong \sum_n f_n p_{\mathcal{N}}\left(\boldsymbol{r}_{\parallel},t|D_{\parallel}^{(n)}\right) \qquad \sum_n f_n = 1$$

$$p_{\mathcal{N}}(\boldsymbol{r}_{\parallel},t|D_{\parallel}) \equiv (4\pi D_{\parallel} t)^{-1} e^{-r_{\parallel}^2/4D_{\parallel}t}$$

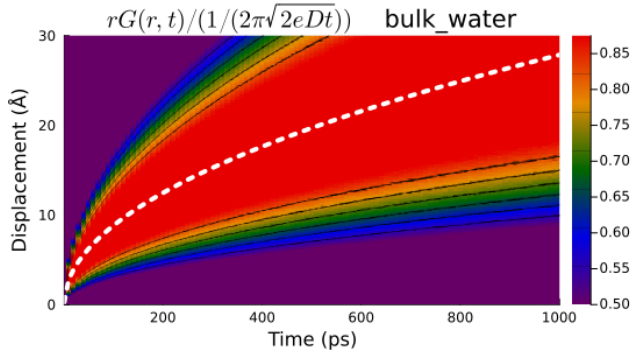
$$f(\boldsymbol{r}_{\parallel},t) \equiv \frac{r_{\parallel} p(\boldsymbol{r}_{\parallel},t)}{\sigma\, p_{\mathcal{N}}(\sigma,t|\sigma)}\Big|_{\sigma=\sqrt{2\langle D_{\parallel}\rangle t}}$$

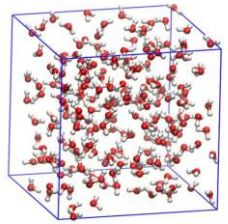


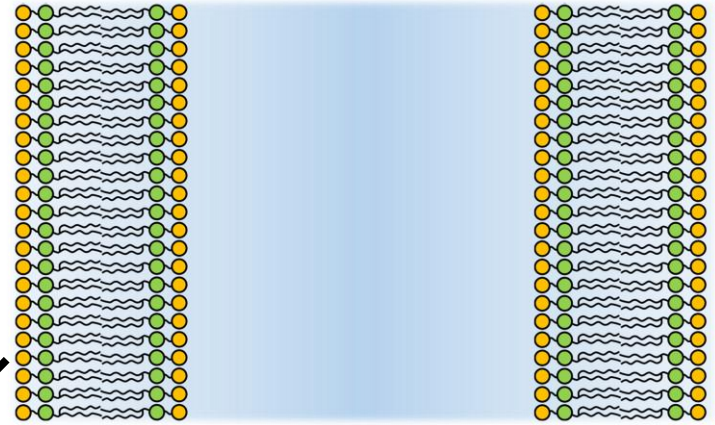


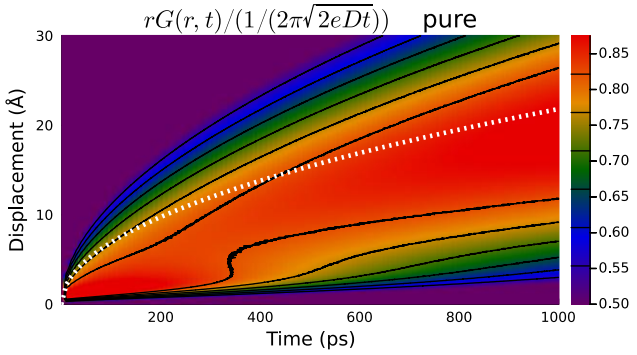


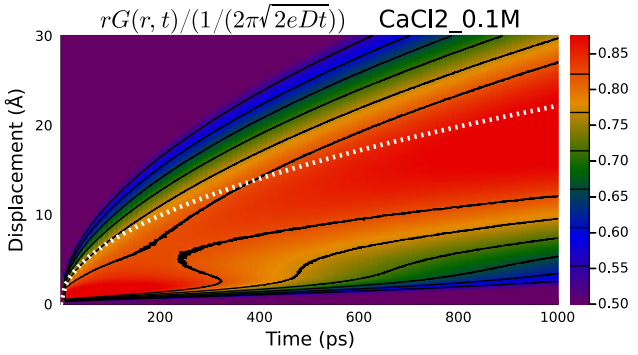
SI Result 2. Lateral Displacement Distribution

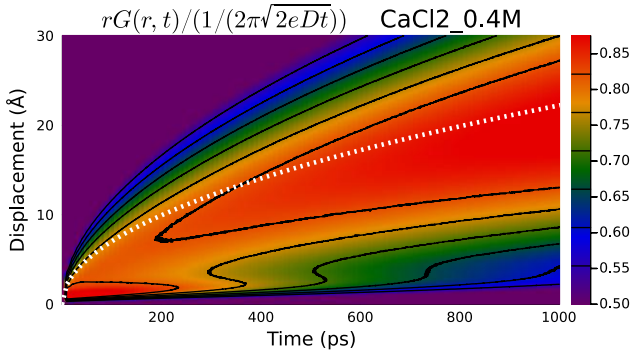


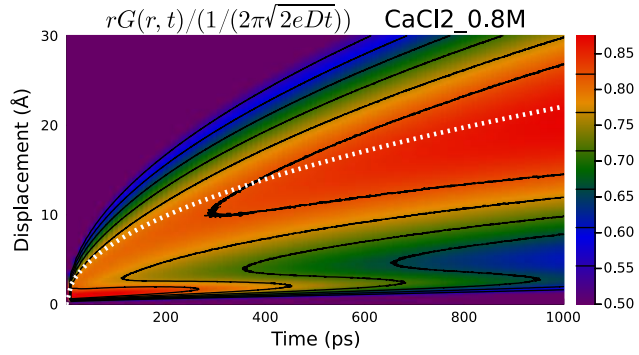


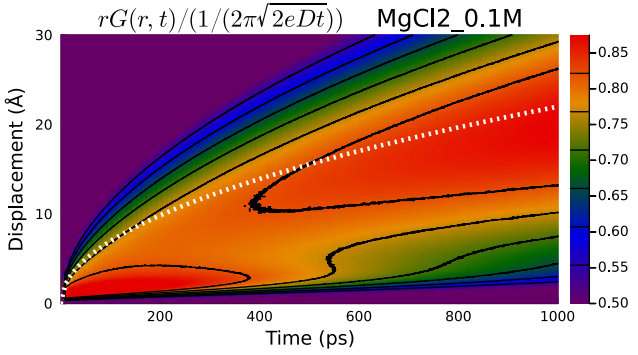


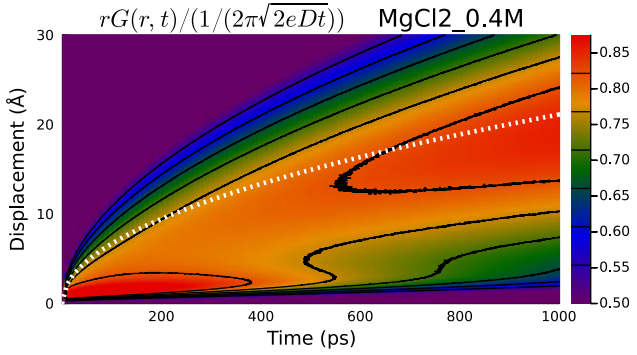


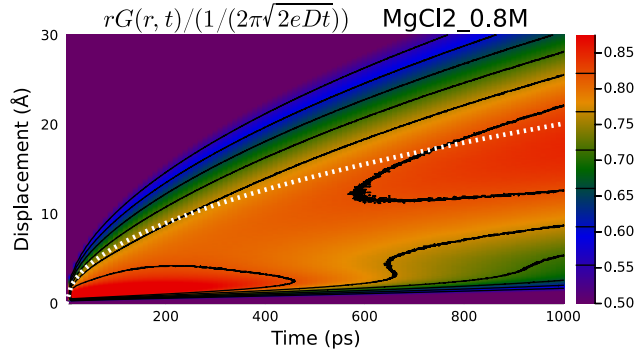












..... $\sqrt{2D_{\parallel}t}$

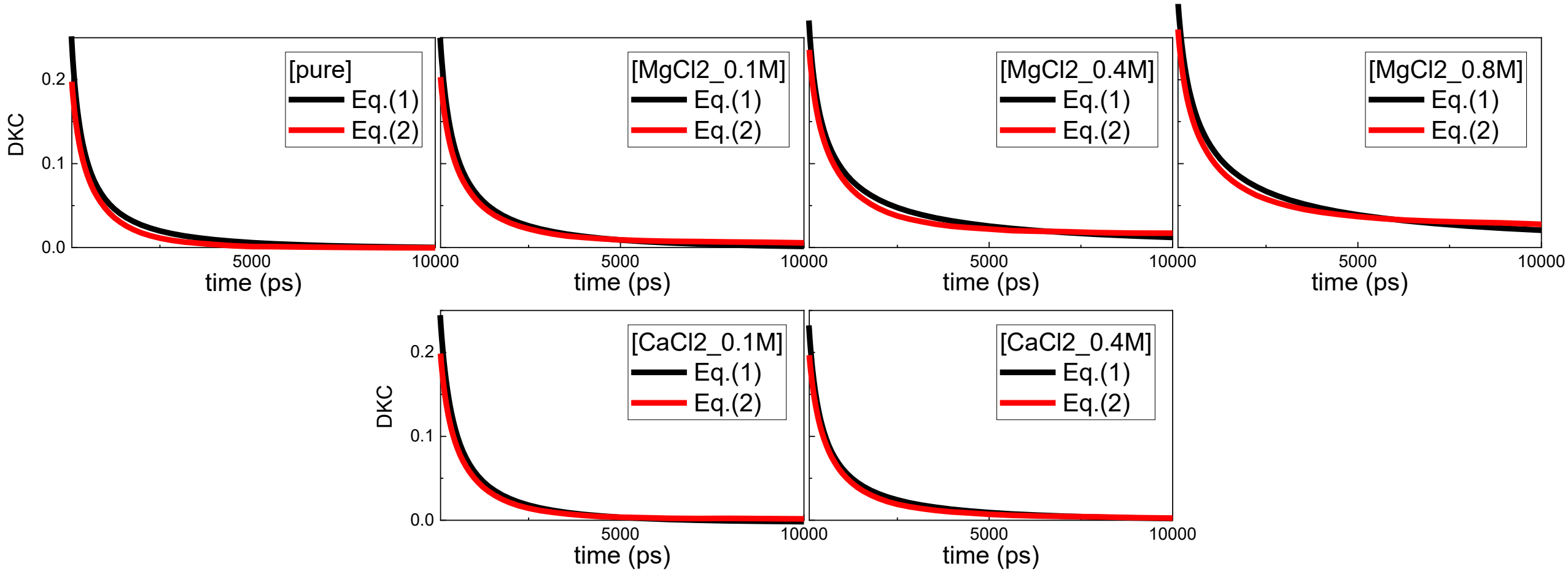
SI Result 4. Diffusion Kernel Correlation

$$C_{\mathcal{D}_\parallel}(t) = \int d\mathbf{\Gamma} \int d\mathbf{\Gamma}_0 \frac{\delta\widehat{\mathcal{D}}_\parallel(\mathbf{\Gamma}, s)}{\langle\widehat{\mathcal{D}}_\parallel(s)\rangle} \hat{G}(\Gamma, s|\Gamma_0) \frac{\delta\widehat{\mathcal{D}}_\parallel(\mathbf{\Gamma}_0, s)}{\langle\widehat{\mathcal{D}}_\parallel(s)\rangle} P_{st}(\mathbf{\Gamma}_0) \quad (1)$$

$$C_{\mathcal{D}_\parallel}(t) \cong \eta_{D_\parallel}^2 \phi_{D_\parallel}(t) = \sum_n \sum_m \frac{\delta D_\parallel(n)}{\langle D_\parallel\rangle} G^{(d)}(n, t|m) \frac{\delta D_\parallel(m)}{\langle D_\parallel\rangle} P_{st}(m) \quad (2)$$

From MSD & NGP

From $G^{(d)}(n, t|m)$ and $D_\parallel(n)$ (Umbrella Sampling)



SI Result 5. Experimental result

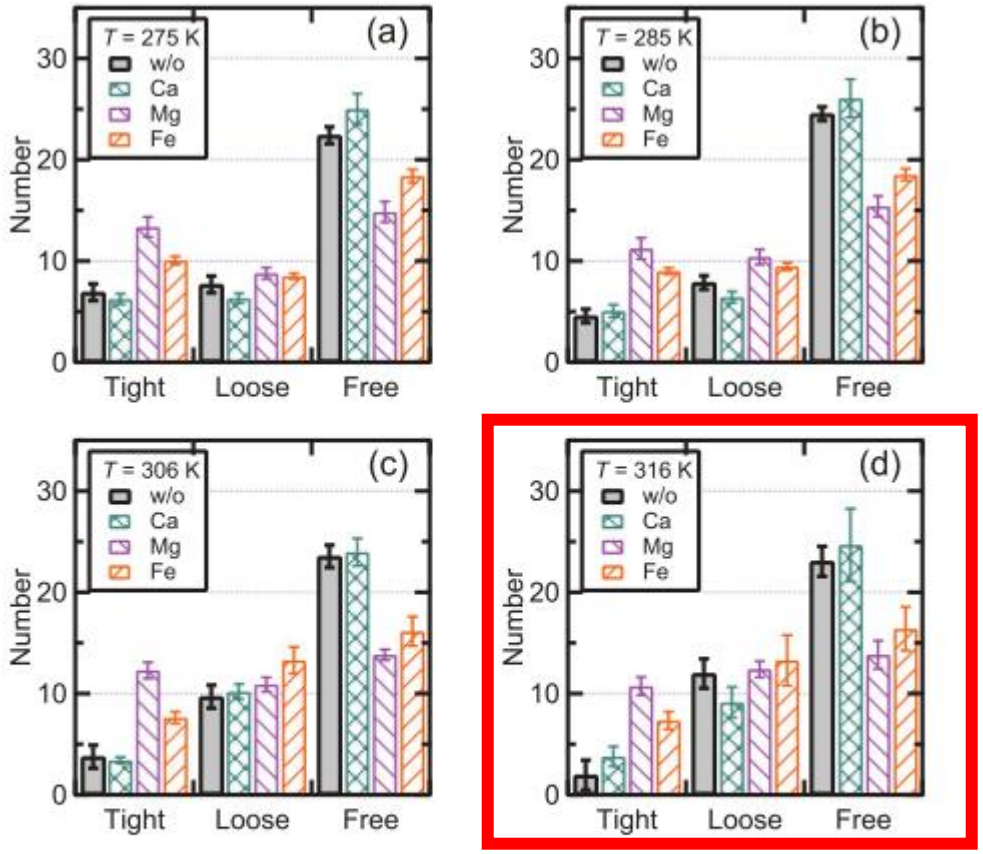


FIG. 3. Temperature dependence of the numbers of free water molecules, loosely bound water molecules, and tightly bound water molecules for *d*67DMPC–37H_2O (gray), *d*67DMPC–37H_2O–0.25$CaCl_2$ (green), *d*67DMPC–37H_2O–0.25$MgCl_2$ (purple), and *d*67DMPC–37H_2O–0.25$FeCl_2$ (orange).

Quasi-elastic neutron scattering study of the effects of metal cations on the hydration water between phospholipid bilayers

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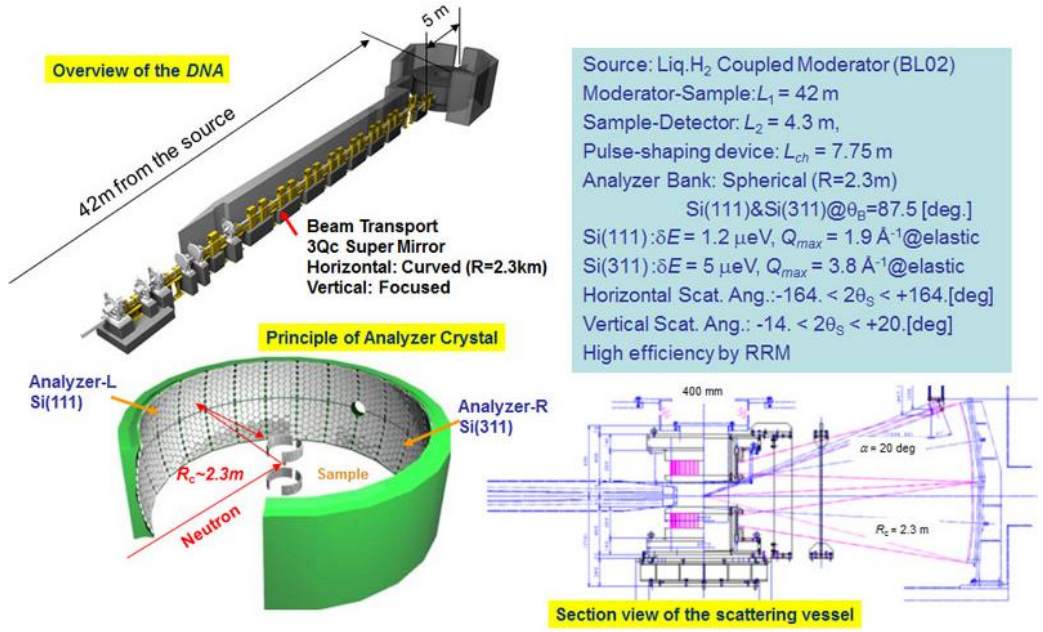
H. Seto[1,a)] and T. Yamada[2,b)]

AFFILIATIONS

[1]Institute of Materials Structure Science/J-PARC Center, High Energy Accelerator Research Organization, Tokai 319-1106, Japan
[2]Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, Tokai 319-1106, Japan

[a)]Author to whom correspondence should be addressed: hideki.seto@kek.jp
[b)]Electronic mail: t_yamada@cross.or.jp



J-PARC MLF BL02 DNA: Dynamic Spectrometer

SI Result 6. PDF of cation, anion