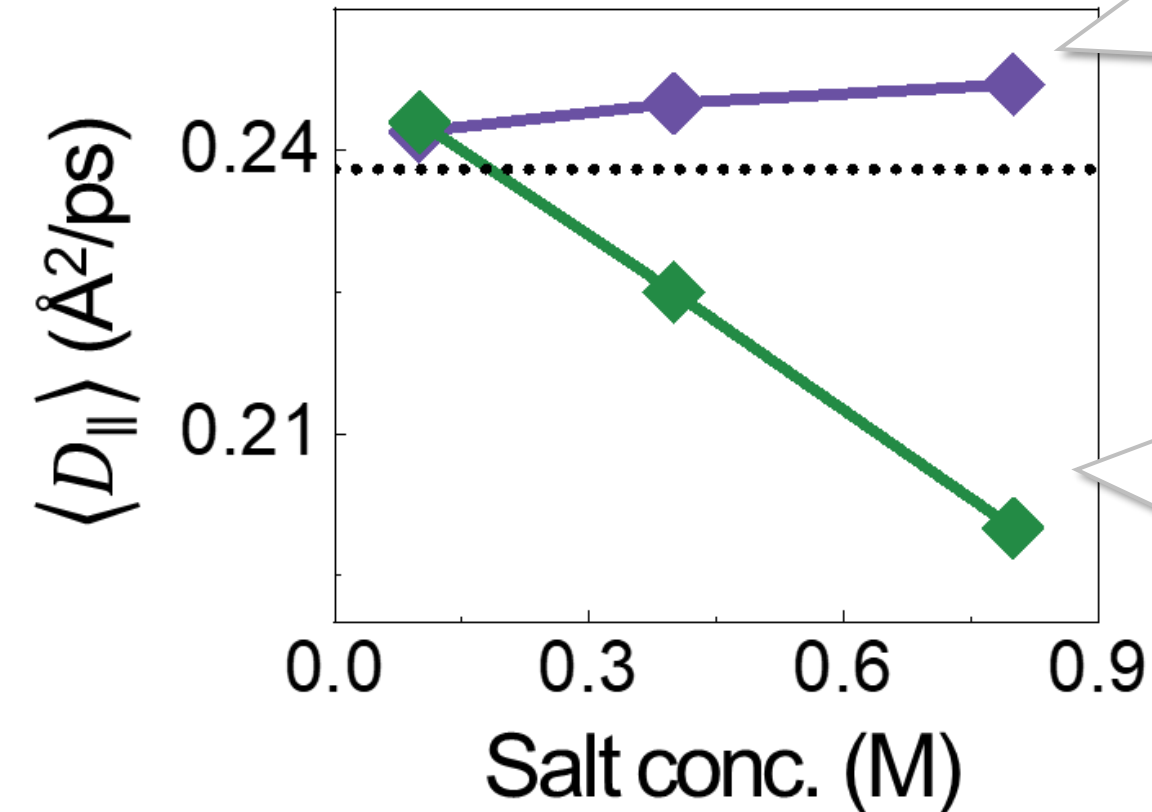
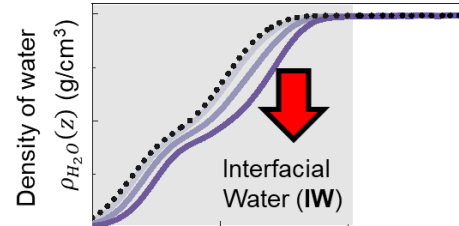


SI Result 1. Mean Diffusion Coefficient

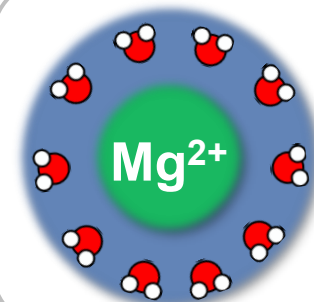
$$\langle D_{\parallel} \rangle = \lim_{t \rightarrow \infty} \frac{\Delta_{2,\parallel}(t)}{t}$$



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



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



$$D_{\parallel}^{\text{H}_2\text{O} \cdots \text{Mg}^{2+}} \ll D_{\parallel}^{\text{H}_2\text{O}}$$

As **Mg²⁺** Conc. Increases,
fraction of **bound water** increases.

SI Result 2. Lateral Displacement Distribution

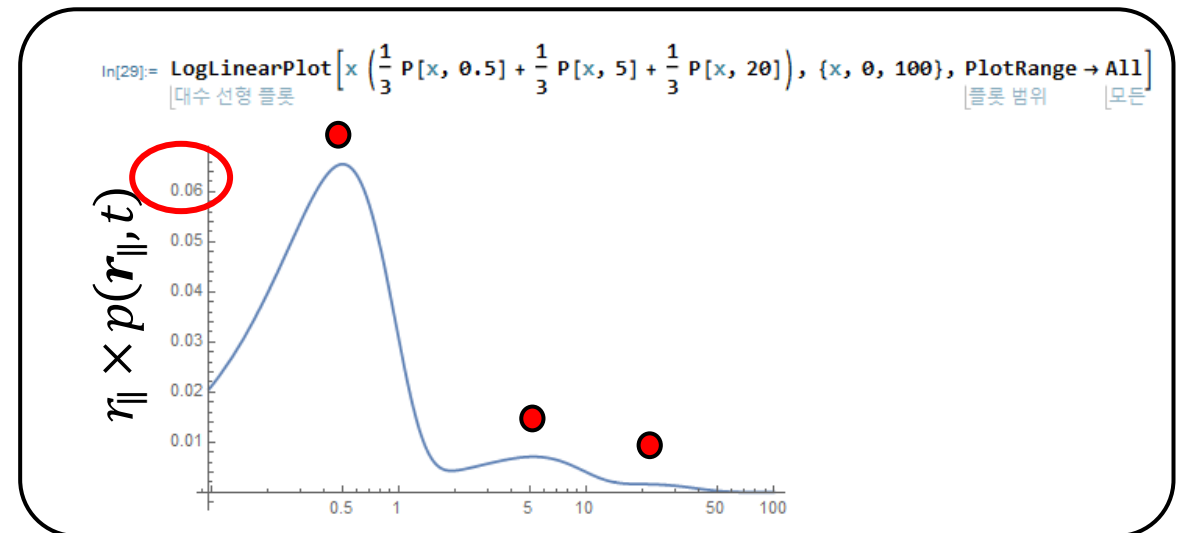
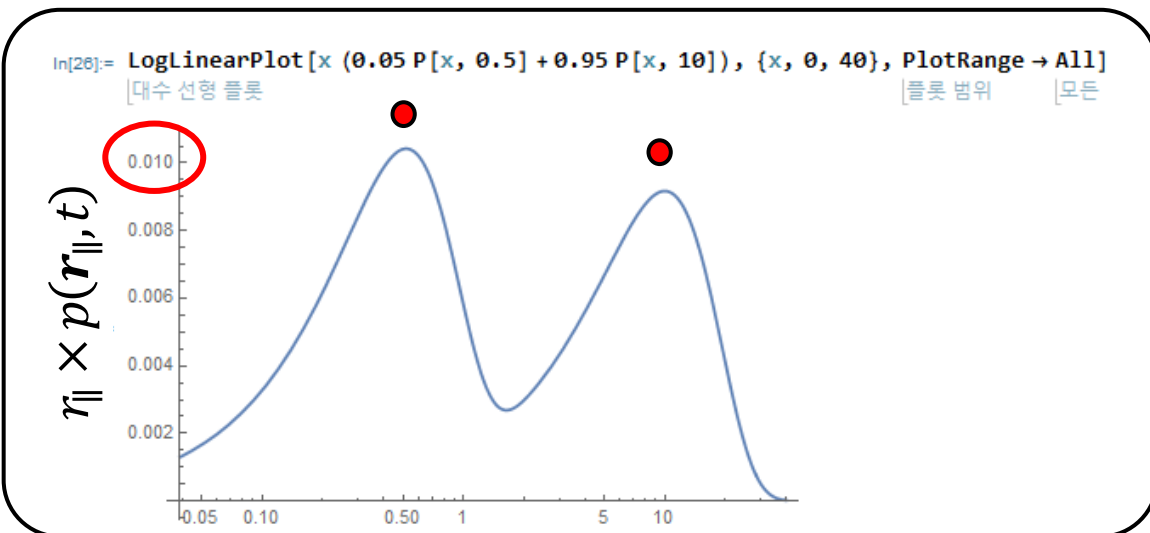
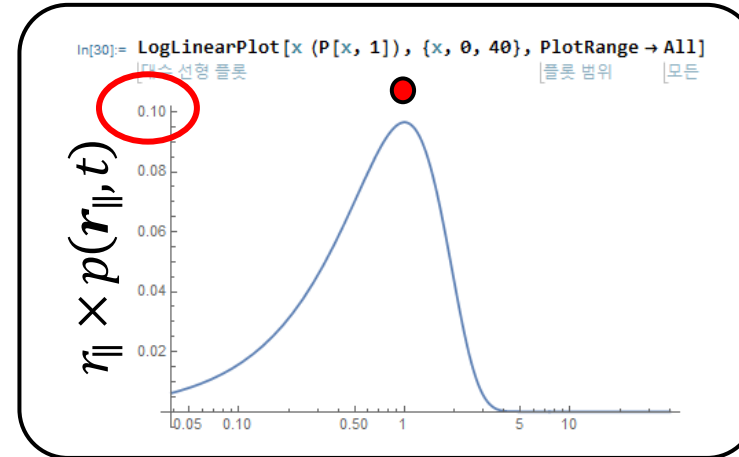
$$p(\mathbf{r}_{\parallel}, t) \cong \sum_n f_n p_{\mathcal{N}}(\mathbf{r}_{\parallel}, t | D_{\parallel}^{(n)}) \quad \sum_n f_n = 1$$

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

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

$$\text{In[2]:= } P[x_ , \sigma_] := (2 \pi \sigma^2)^{-1} \text{Exp}[-x^2 / (2 \sigma^2)]$$

[지수 함수]

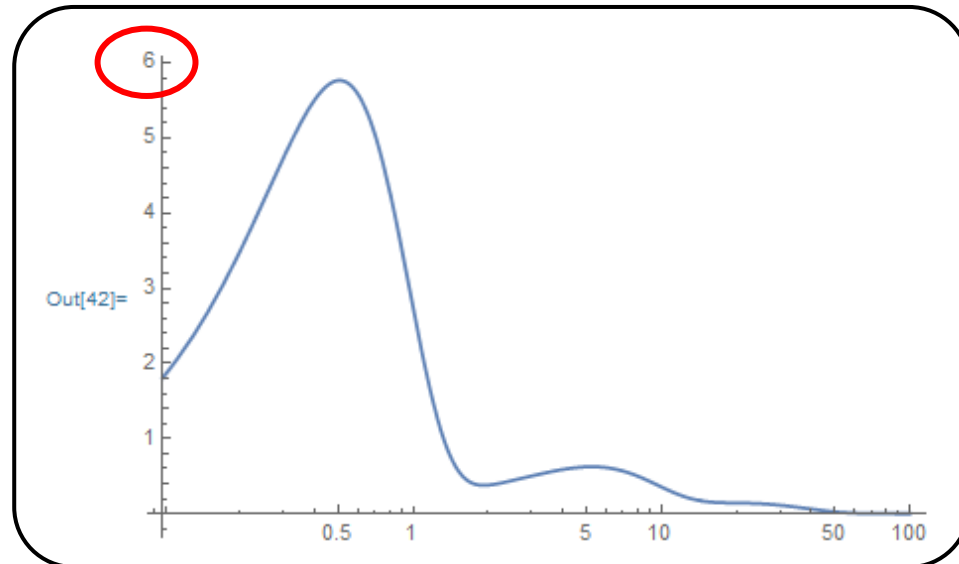
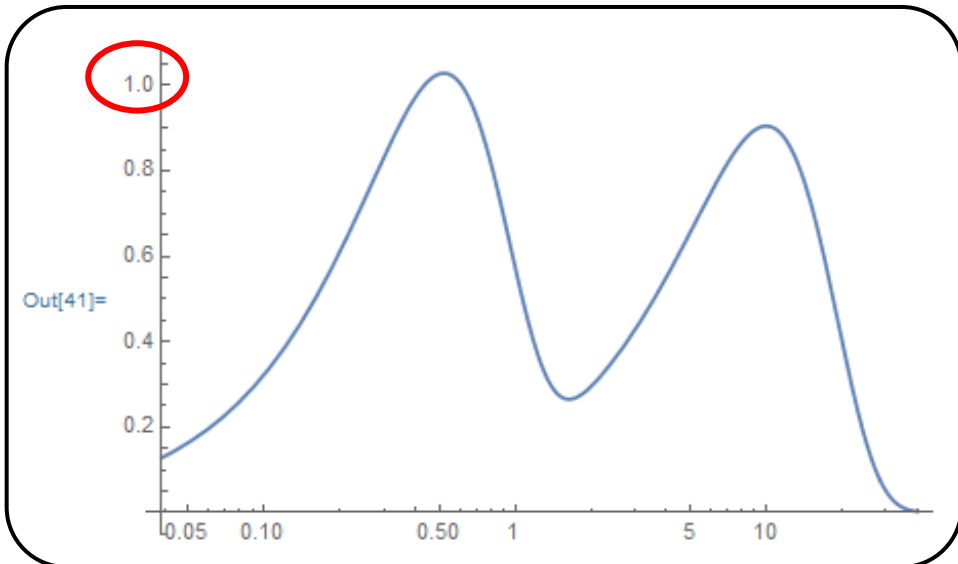
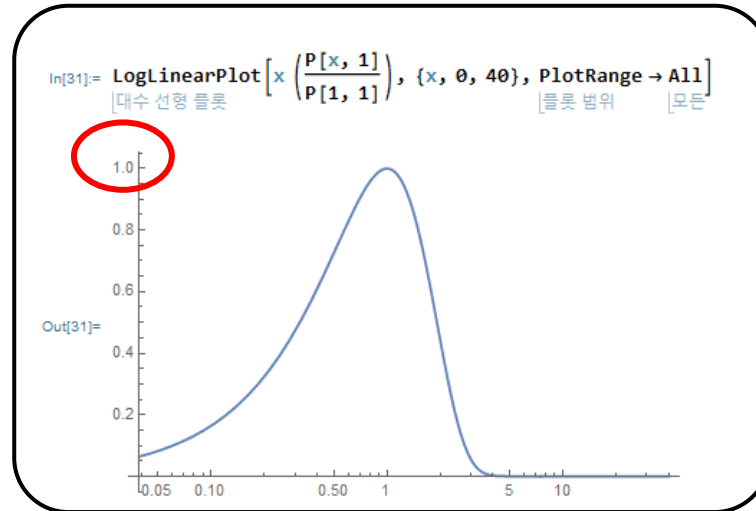


SI Result 2. Lateral Displacement Distribution

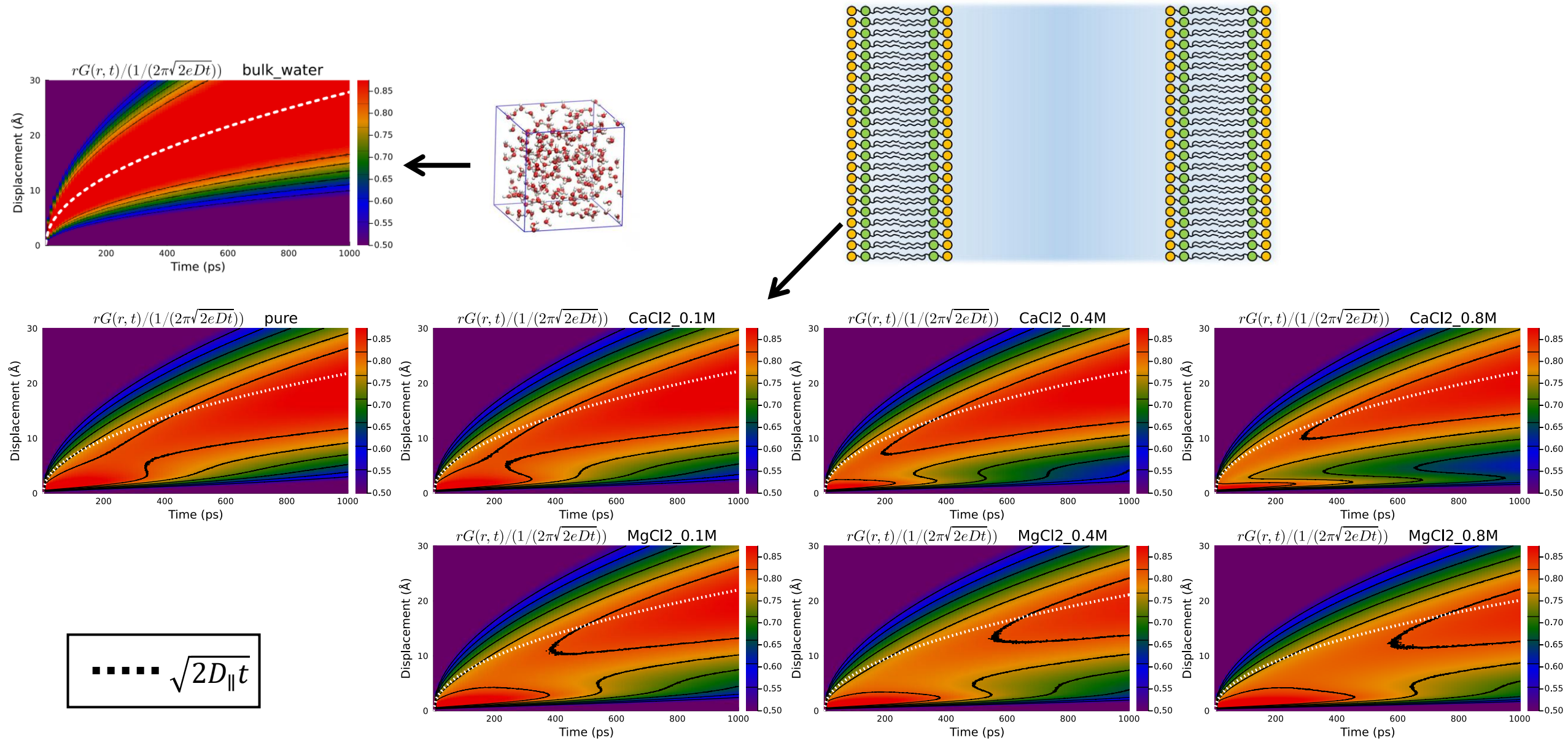
$$p(\mathbf{r}_{\parallel}, t) \cong \sum_n f_n p_{\mathcal{N}}(\mathbf{r}_{\parallel}, t | D_{\parallel}^{(n)}) \quad \sum_n f_n = 1$$

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

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



SI Result 2. Lateral Displacement Distribution



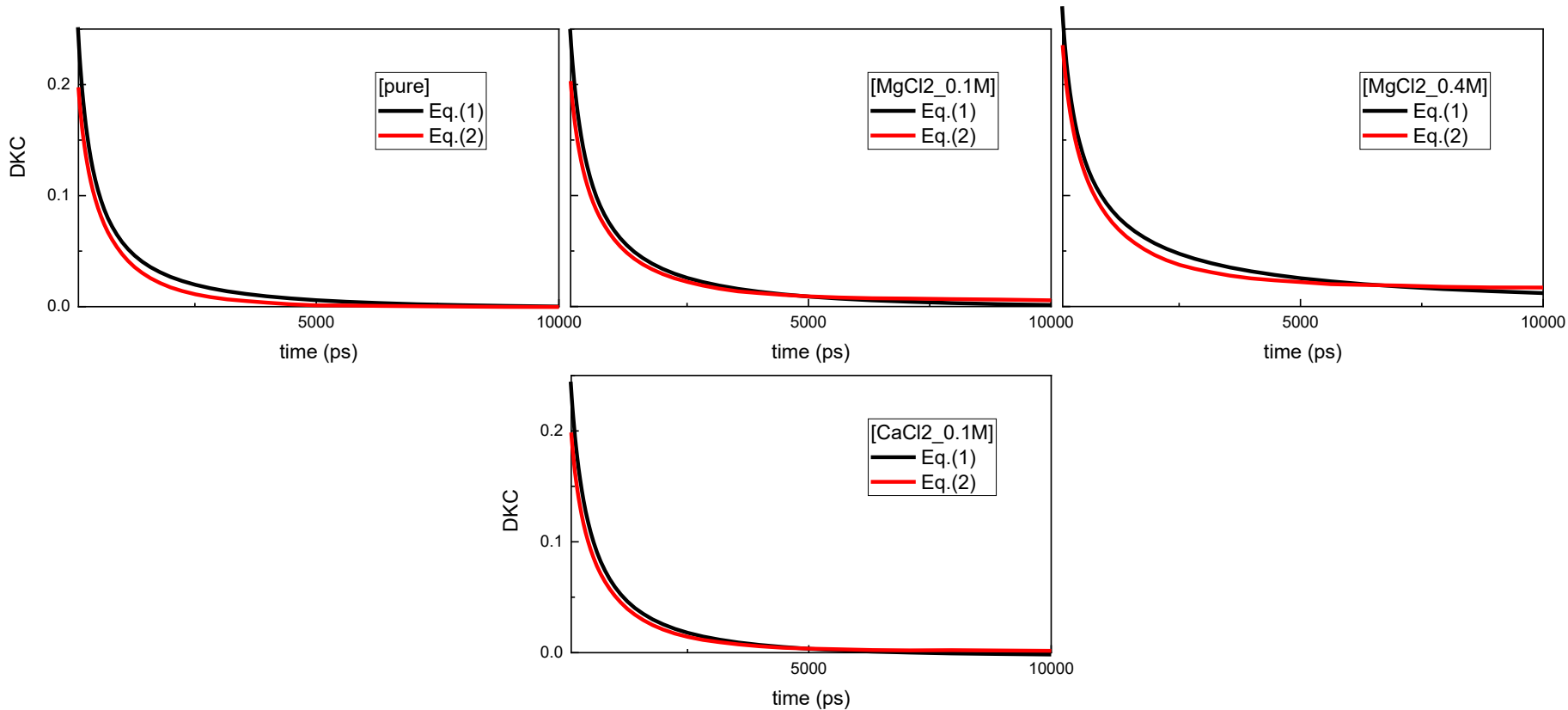
SI Result 4. Diffusion Kernel Correlation

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

From MSD & NGP

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

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



SI Result 5. Experimental result

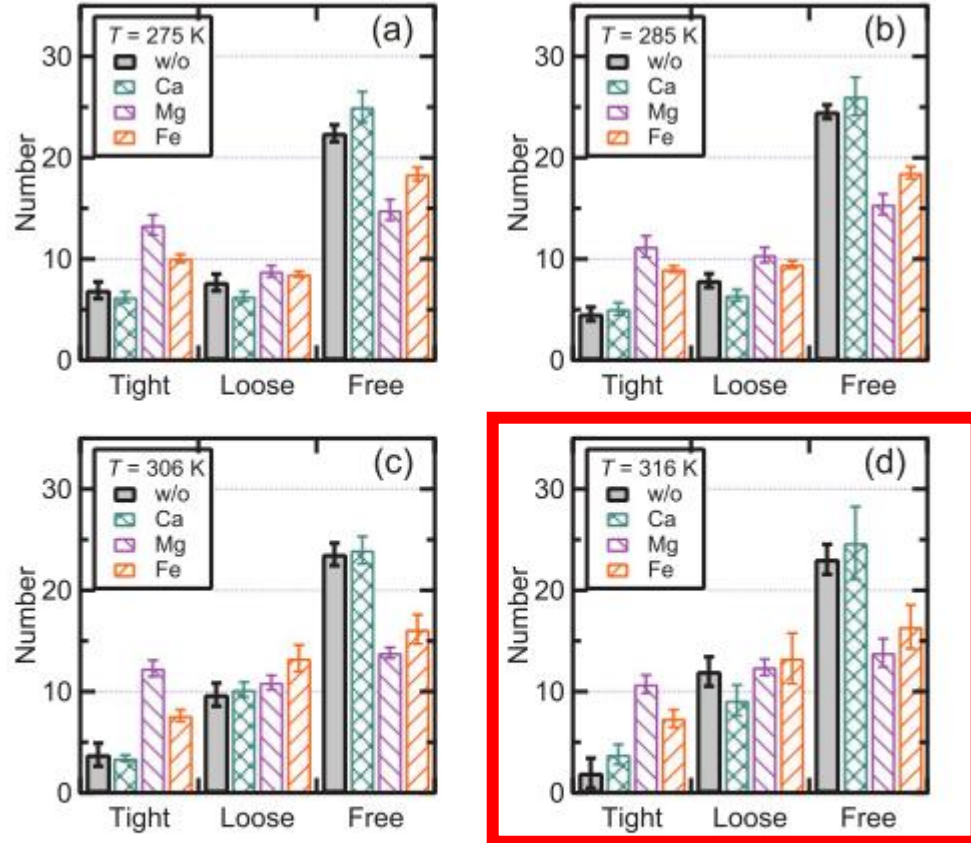


FIG. 3. Temperature dependence of the numbers of free water molecules, loosely bound water molecules, and tightly bound water molecules for d67DMPC-37H₂O (gray), d67DMPC-37H₂O-0.25CaCl₂ (green), d67DMPC-37H₂O-0.25MgCl₂ (purple), and d67DMPC-37H₂O-0.25FeCl₂ (orange).

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

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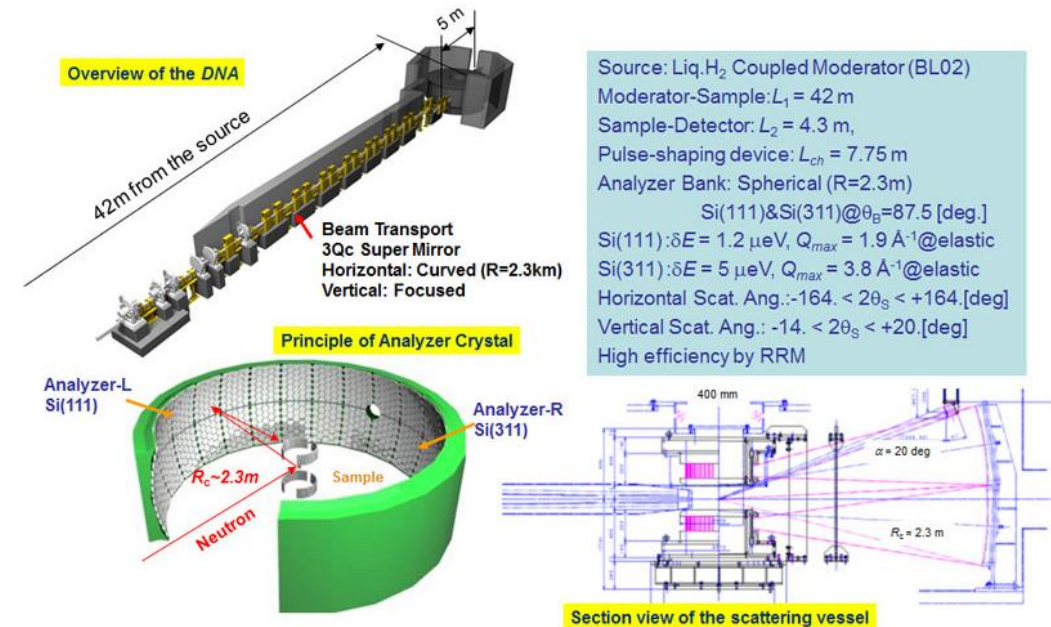
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J-PARC MLF BL02 DNA: Dynamic Spectrometer

SI Result 6. PDF of cation, anion

MgCl₂

0.1M

0.4M

0.8M

CaCl₂

0.1M

0.4M

0.8M

Pure water

■ ■ ■

