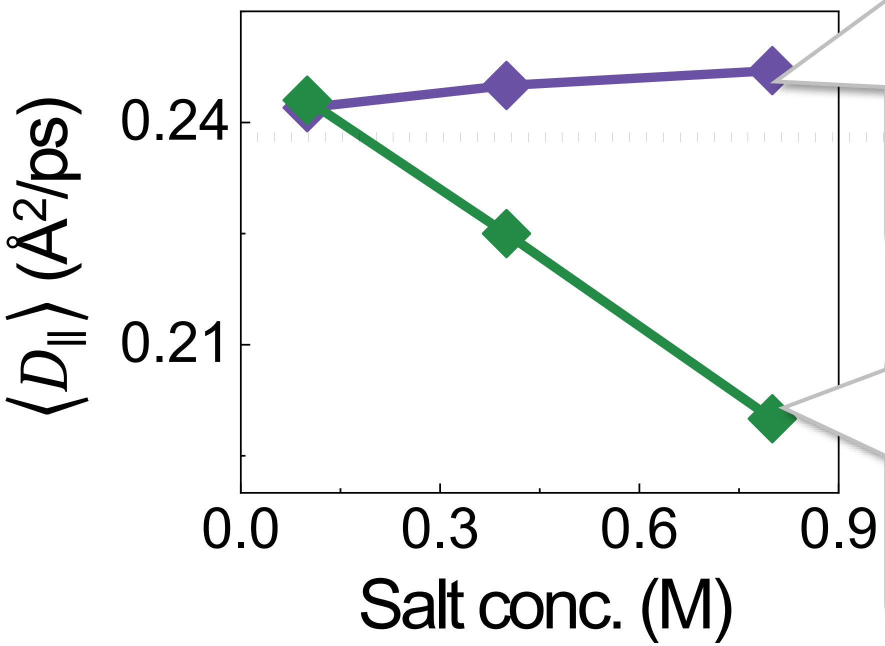
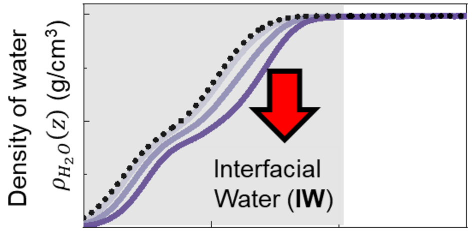
# SI Result 1. Mean Diffusion Coefficient

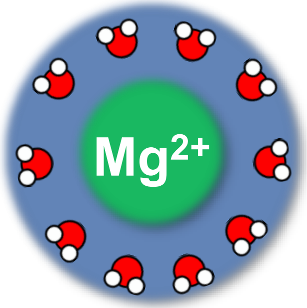
$$\langle D_\parallel \rangle = \lim_{t\to\infty} \frac{\Delta_{2,\parallel}(t)}{t}$$




**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.**

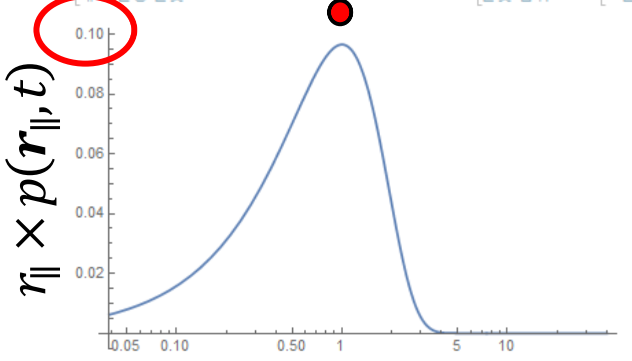
# SI Result 2. Lateral Displacement Distribution

$$p(\boldsymbol{r}_\parallel, t) \cong \sum_n f_n p_{\mathcal{N}}\left(\boldsymbol{r}_\parallel, t | D_\parallel^{(n)}\right) \qquad \sum_n f_n = 1 \qquad p_{\mathcal{N}}(\boldsymbol{r}_\parallel, t|D_\parallel) \equiv (4\pi D_\parallel t)^{-1} e^{-r_\parallel^2/4D_\parallel t}$$

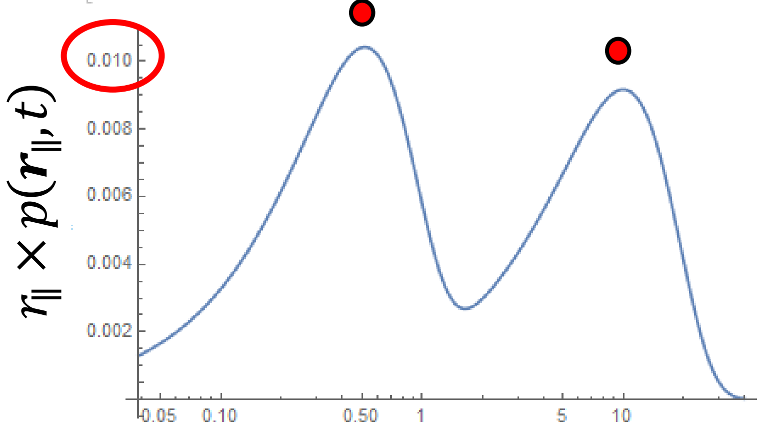
$$r_\parallel \times p_{\mathcal{N}}(\boldsymbol{r}_\parallel, t|D_\parallel) \rightarrow \text{ maximum at } r_\parallel = \sigma = \sqrt{2D_\parallel t}$$

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

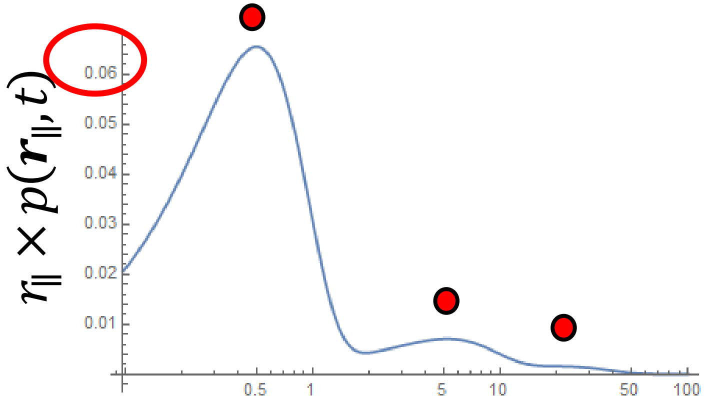
```
In[30]:= LogLinearPlot[x (P[x, 1]), {x, 0, 40}, PlotRange → All]
         대수 선형 플롯                               플롯 범위   모든
```




```
In[26]:= LogLinearPlot[x (0.05 P[x, 0.5] + 0.95 P[x, 10]), {x, 0, 40}, PlotRange → All]
         대수 선형 플롯                                              플롯 범위   모든
```




```
In[29]:= LogLinearPlot[x (1/3 P[x, 0.5] + 1/3 P[x, 5] + 1/3 P[x, 20]), {x, 0, 100}, PlotRange → All]
         대수 선형 플롯                                                       플롯 범위   모든
```



# SI Result 2. Lateral Displacement Distribution

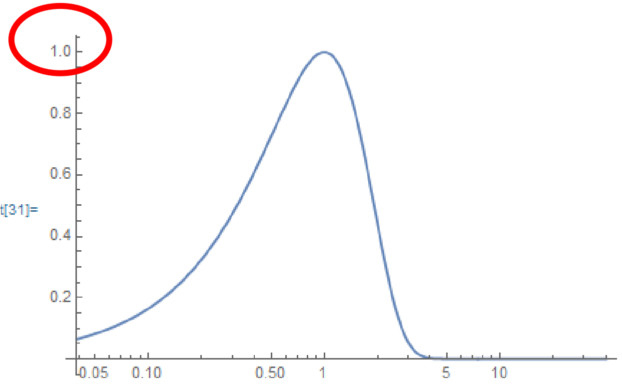
$$p(\boldsymbol{r}_\parallel,t) \cong \sum_n f_n p_{\mathcal{N}}\left(\boldsymbol{r}_\parallel, t \middle| D_\parallel^{(n)}\right) \qquad \sum_n f_n = 1$$

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

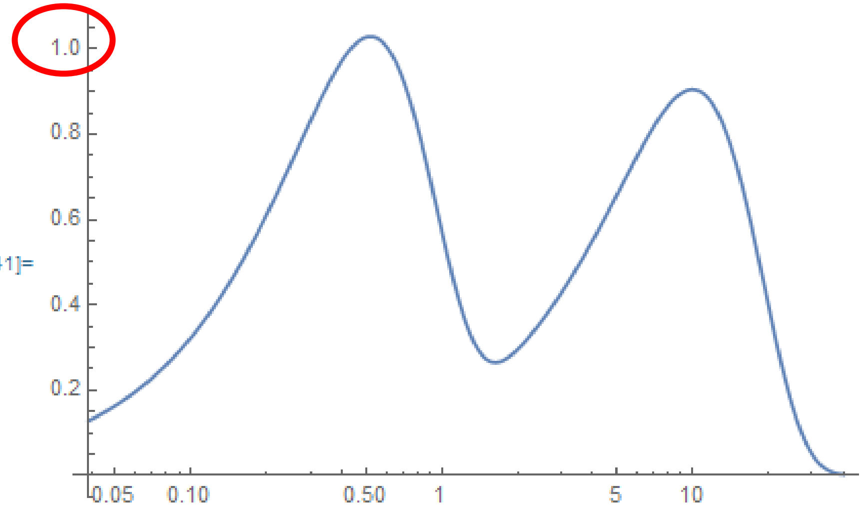
$$f(\boldsymbol{r}_\parallel,t) \equiv \left.\frac{r_\parallel p(\boldsymbol{r}_\parallel,t)}{\sigma p_{\mathcal{N}}(\sigma,t|\sigma)}\right|_{\sigma=\sqrt{2\langle D_\parallel\rangle t}}$$

```
In[31]:= LogLinearPlot[x (P[x, 1] / P[1, 1]), {x, 0, 40}, PlotRange → All]
          [대수 선형 플롯                                  [플롯 범위  [모든
```

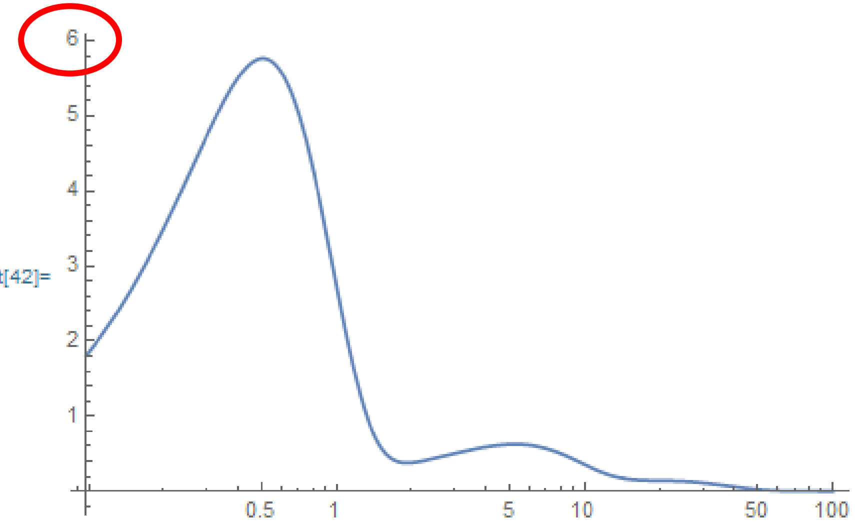
Out[31]=



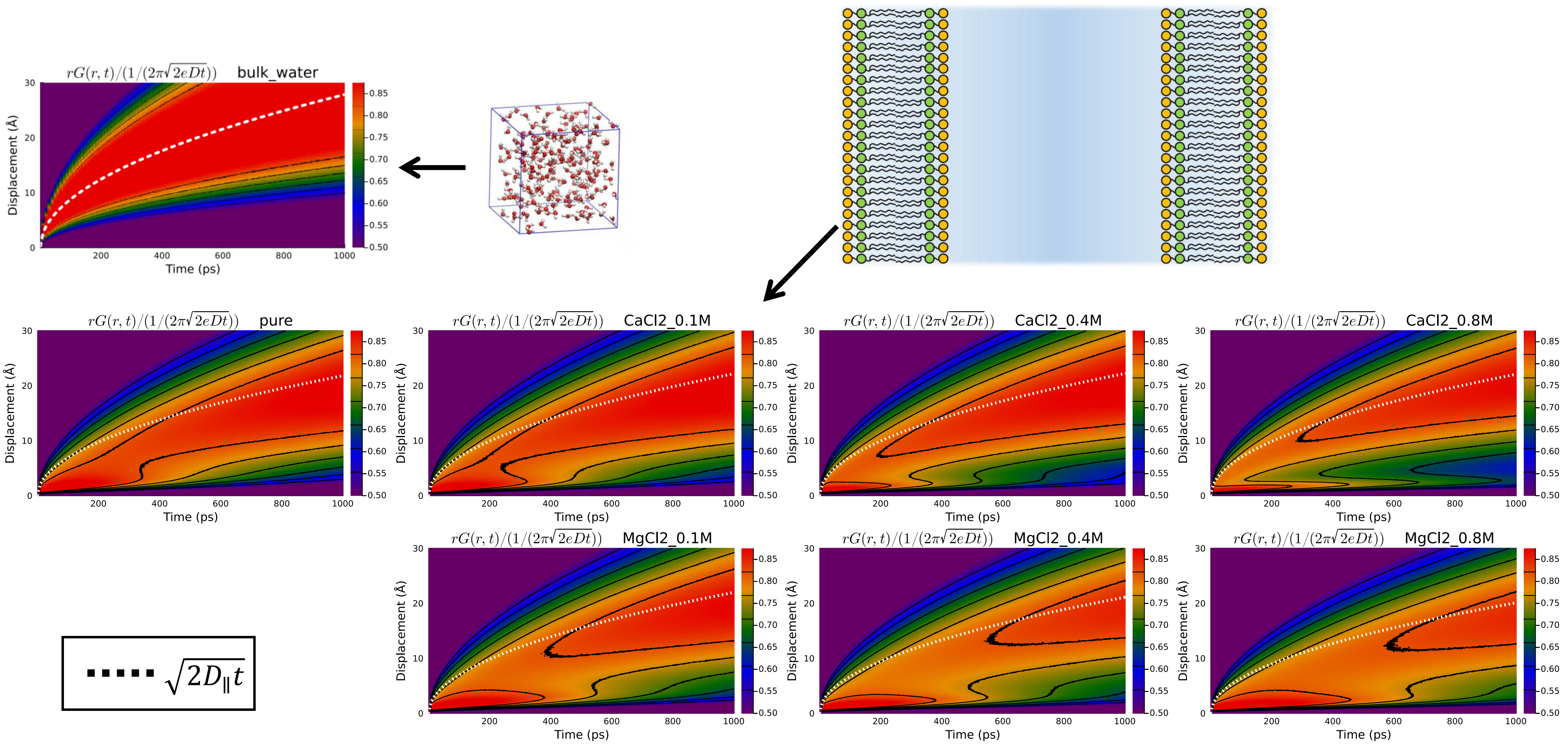

Out[41]=




Out[42]=



# SI Result 2. Lateral Displacement Distribution



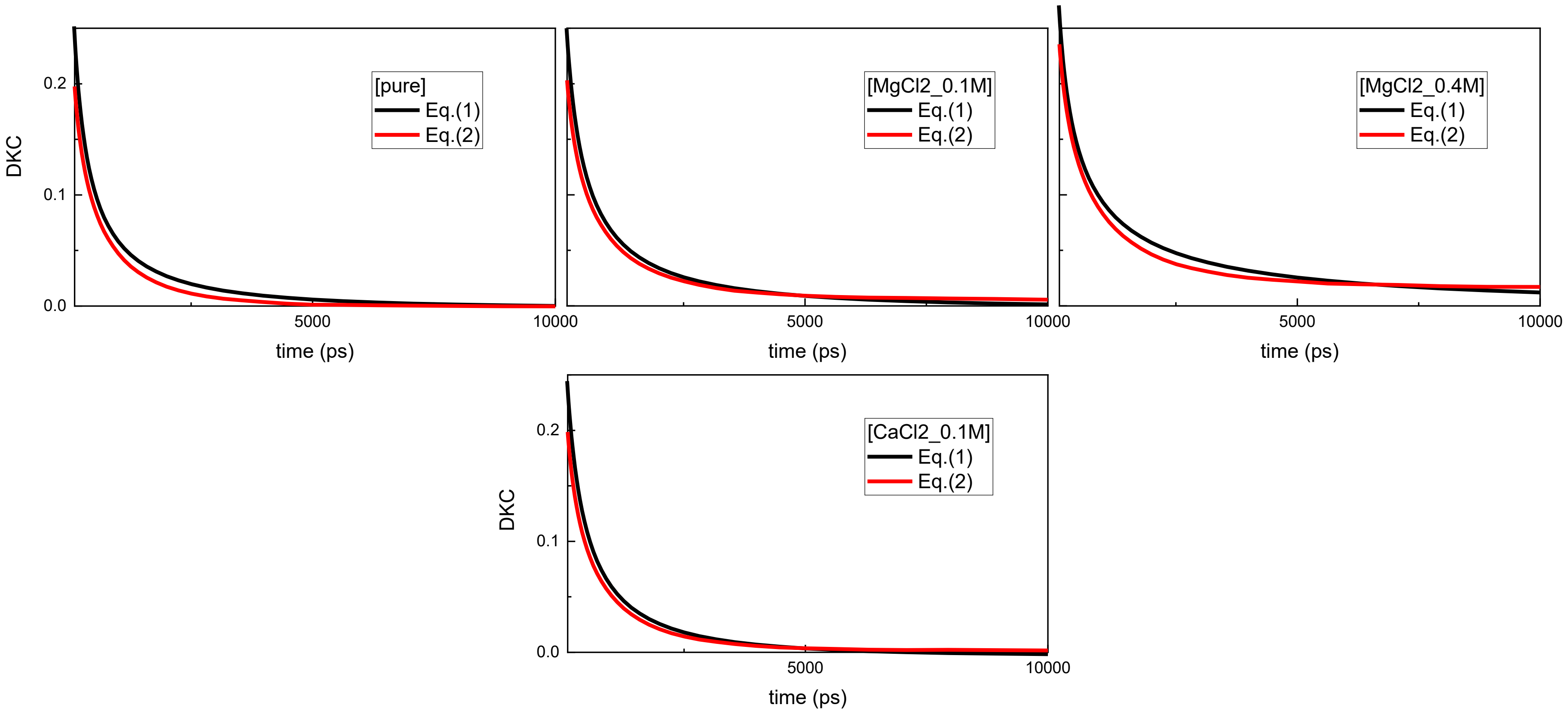
# SI Result 4. Diffusion Kernel Correlation

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

**From MSD & NGP**

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

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



# SI Result 5. Experimental result

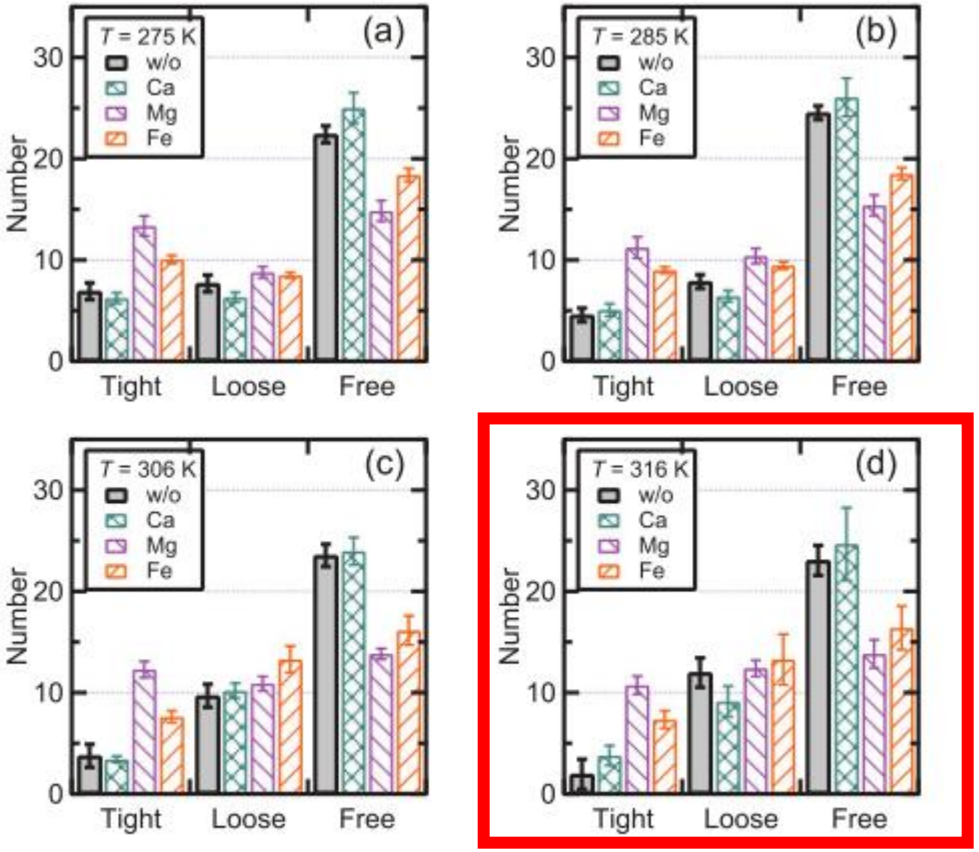



**FIG. 3.** Temperature dependence of the numbers of free water molecules, loosely bound water molecules, and tightly bound water molecules for *d*67DMPC–37$H_2O$ (gray), *d*67DMPC–37$H_2O$–0.25$CaCl_2$ (green), *d*67DMPC–37$H_2O$–0.25$MgCl_2$ (purple), and *d*67DMPC–37$H_2O$–0.25$FeCl_2$ (orange).

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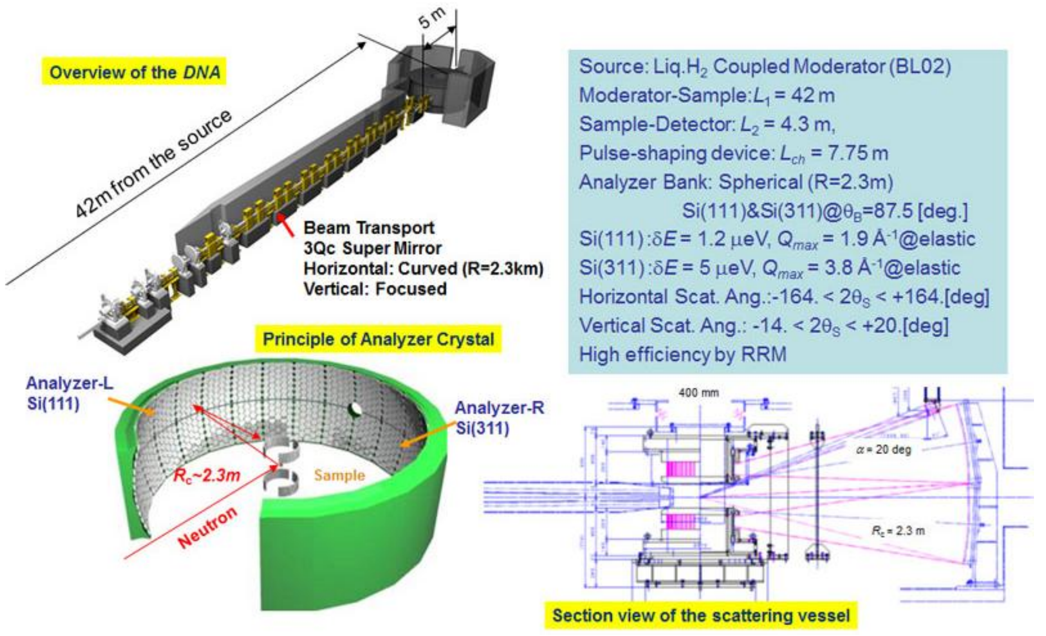


**J-PARC MLF BL02 DNA: Dynamic Spectrometer**

# SI Result 6. PDF of cation, anion