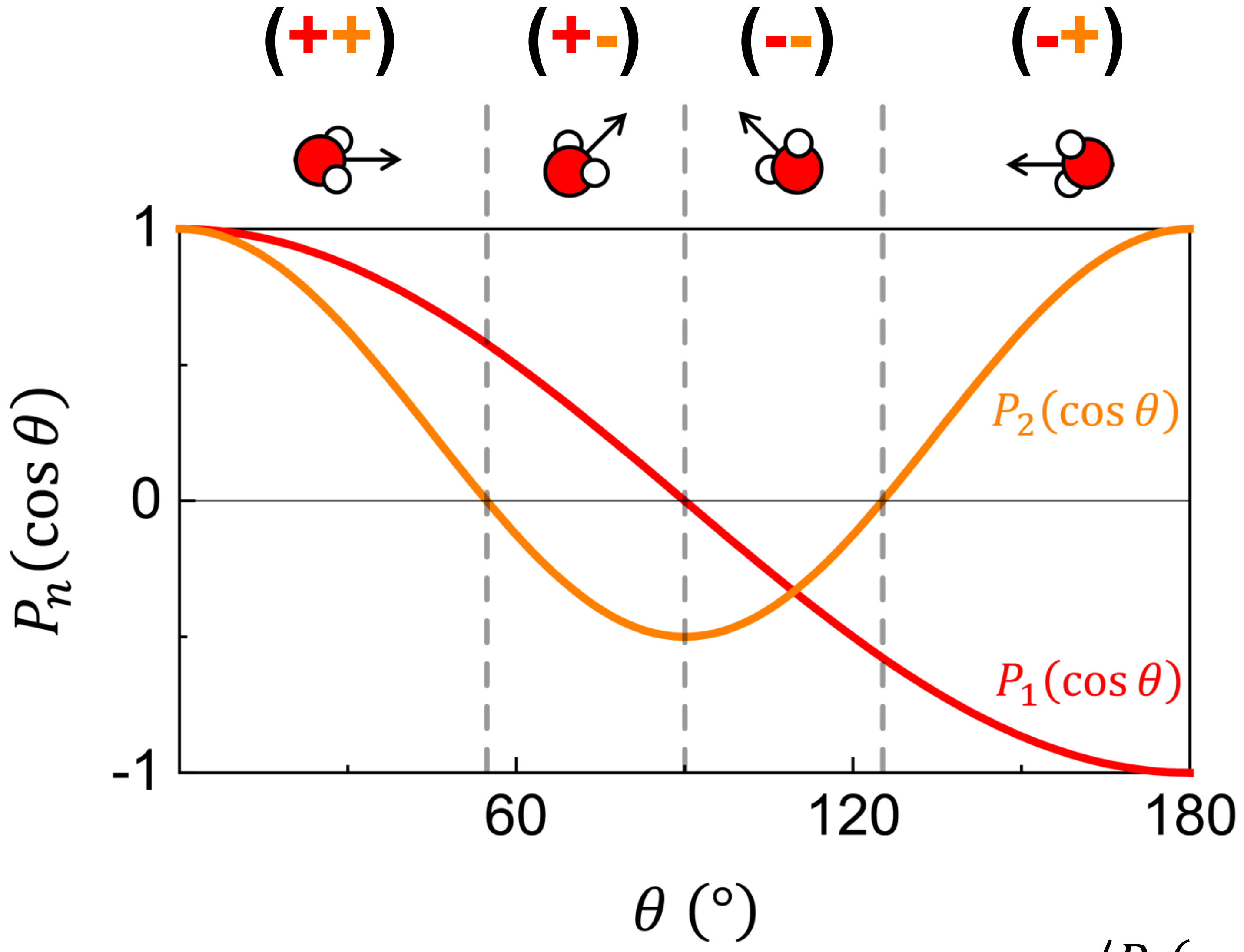
SI Result 1 (a): Legendre Polynomial



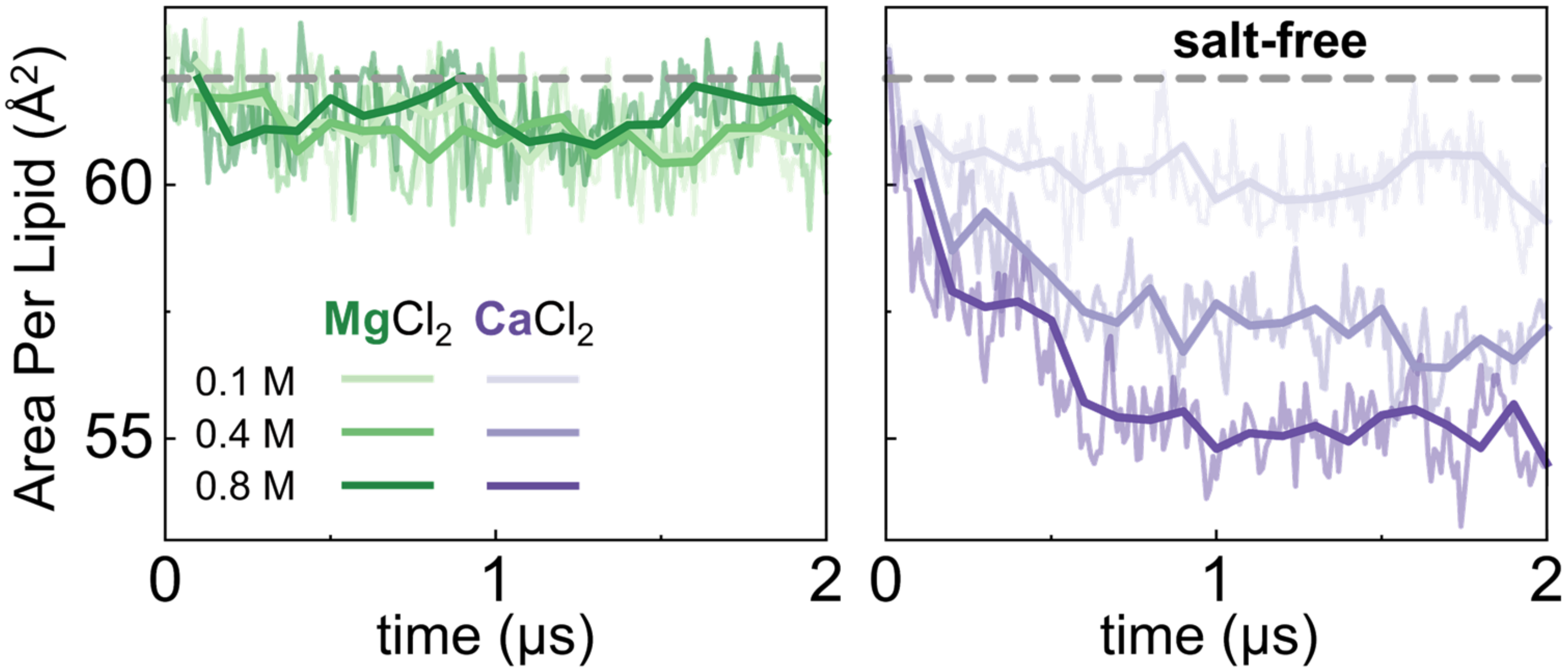
See **Fig. 2 (d)** and **Fig. 2 (e)**

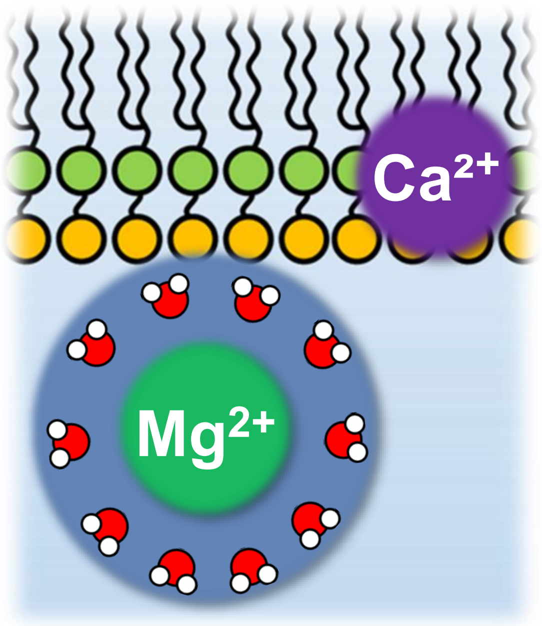
$$P_1(\cos\theta) = \cos\theta$$

$$P_2(\cos\theta) = \left(3\cos^2\theta - 1\right)/2$$

$$\langle P_n(\cos\theta)\rangle(z) = \int_0^{\pi} d\theta \sin\theta \, P_n(\cos\theta) p(\theta, z)$$

SI Result 1 (b): Area per lipid





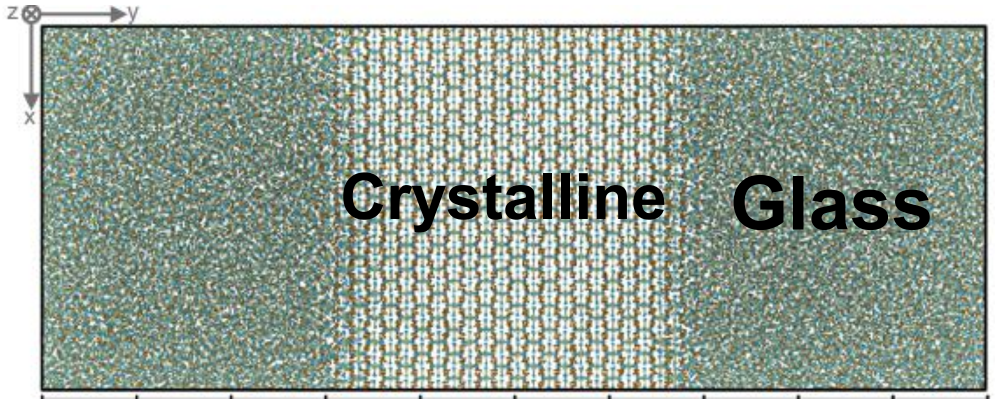
- Mg^{2+} cannot induce membrane condensation due to its **hydration shell** **[7]**.
- Ca^{2+} reduces repulsion between headgroups, inducing **membrane condensation** [7].
- As Conc. of $CaCl_2$ increases, portion of interfacial water (**IW**) of $CaCl_2$ decreases.

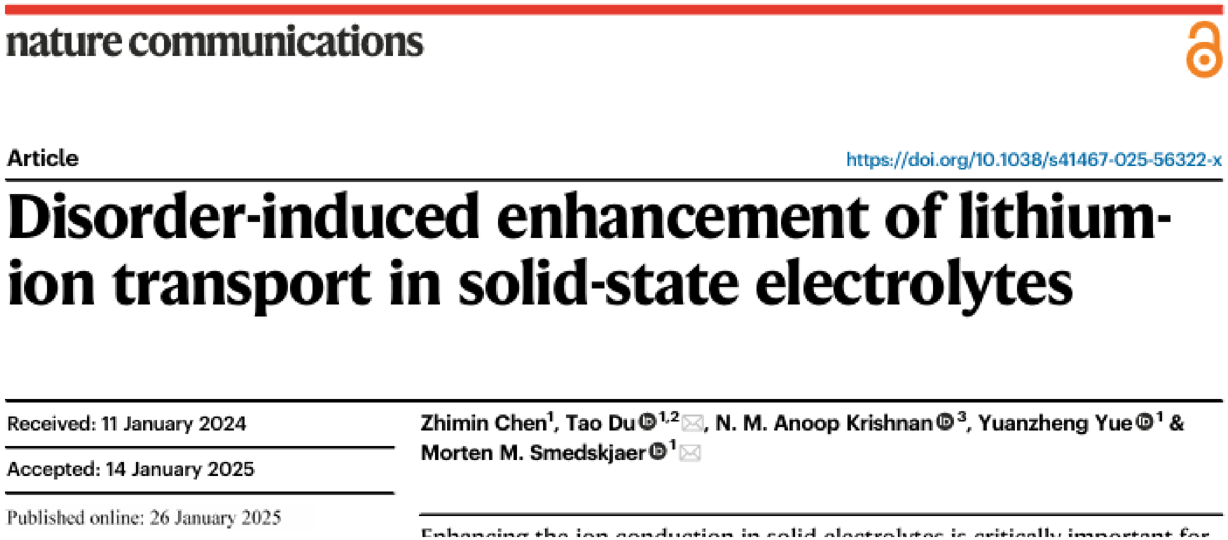
(See $\rho_{H_2O}(z)$ in **Fig. 2 (f)**)

[7] Yi Dong, J. Phys. Chem. Lett., 13, 11237-11244 (2022)

SI Result 1 (c): Lateral Displacement Distribution

Li_3PS_4





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Article

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Disorder-induced enhancement of lithium-ion transport in solid-state electrolytes

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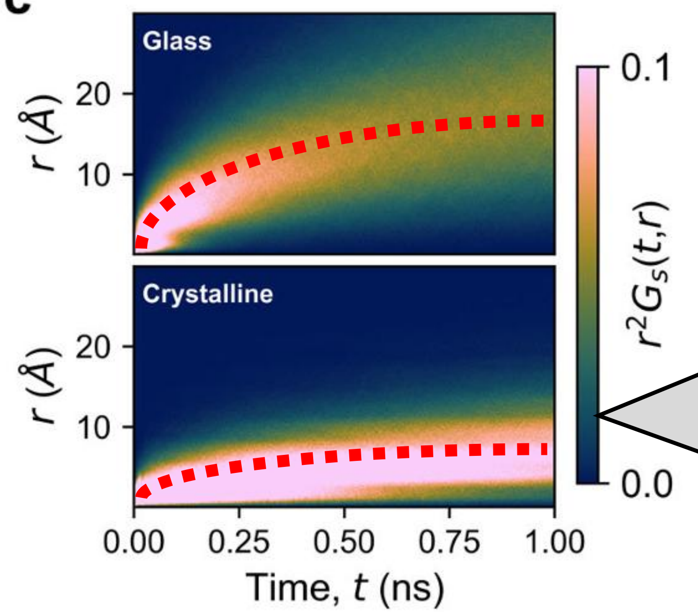
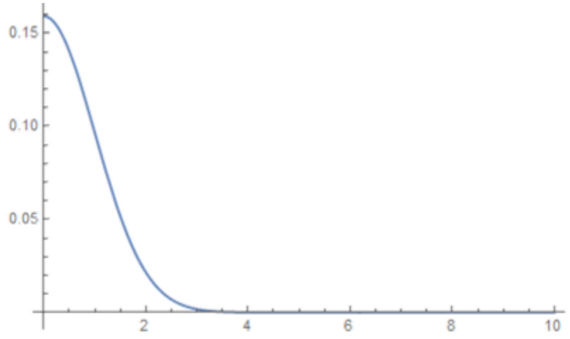
c



$2Dt\sqrt{2}$

Li ions in "Glass" phase diffuse faster than those in the crystalline!!

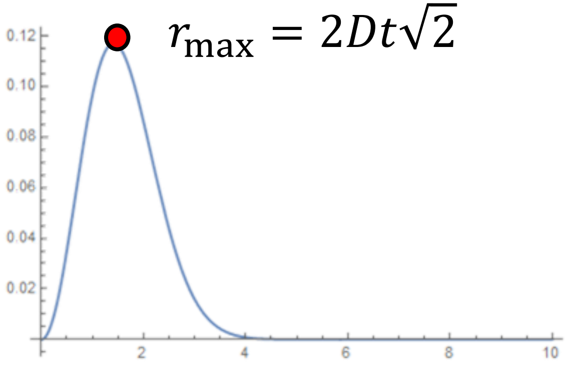
$$G_s(\boldsymbol{r},t) = (4\pi Dt)^{-3/2} e^{-r^2/4Dt}$$



r

$$r^2 G_s(\boldsymbol{r},t)$$

$$r_{\max} = 2Dt\sqrt{2}$$



r

SI Result 1 (c): Lateral Displacement Distribution

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

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

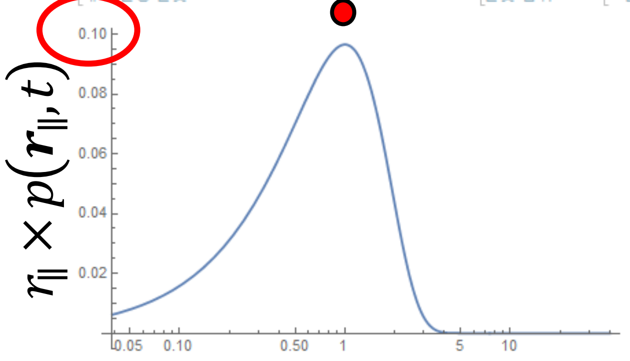
$$r_\parallel \times G_{\mathcal{N}}(\boldsymbol{r}_\parallel, t | D_\parallel) \rightarrow \text{ maximum at } r_\parallel = \sigma = \sqrt{2 D_\parallel t}$$

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

지수 함수

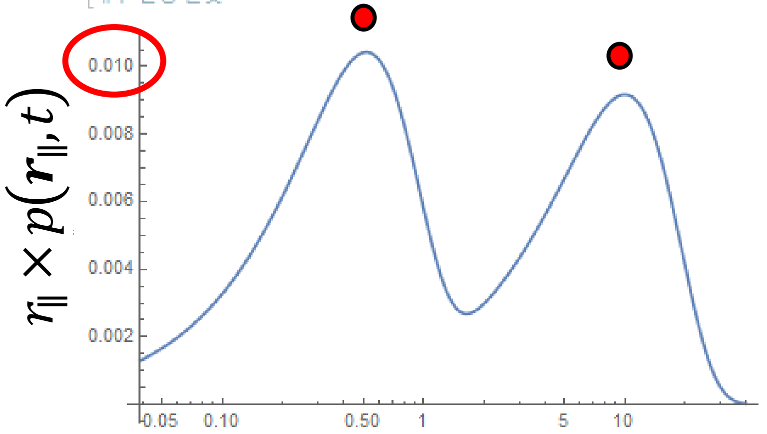
```
In[30]:= LogLinearPlot[x (P[x, 1]), {x, 0, 40}, PlotRange → All]
```

대수 선형 플롯 플롯 범위 모든



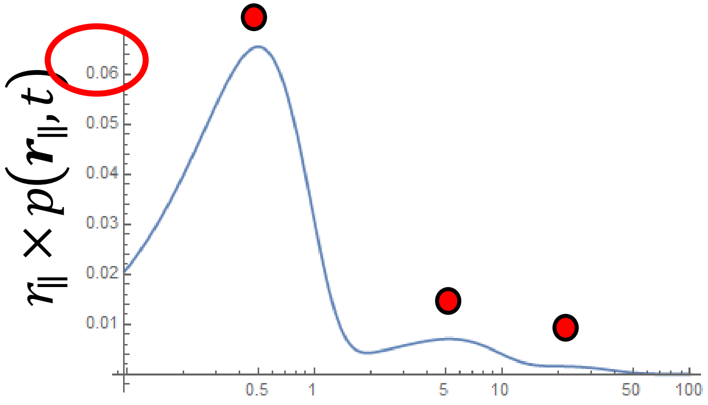

```
In[26]:= LogLinearPlot[x (0.05 P[x, 0.5] + 0.95 P[x, 10]), {x, 0, 40}, PlotRange → All]
```

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 1 (c): Lateral Displacement Distribution

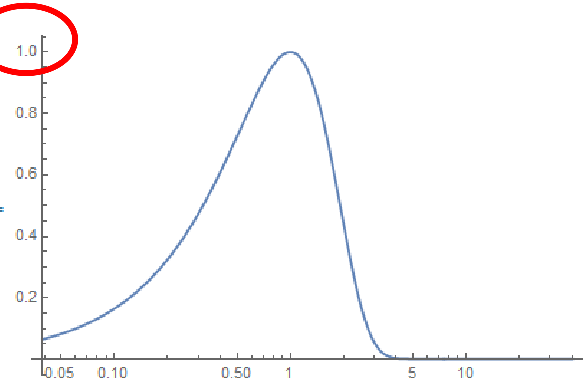
$$G_s(\boldsymbol{r}_\parallel, t) \cong \sum_n f_n G_{\mathcal{N}}\left(\boldsymbol{r}_\parallel, t \middle| D_\parallel^{(n)}\right) \qquad \sum_n f_n = 1$$

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

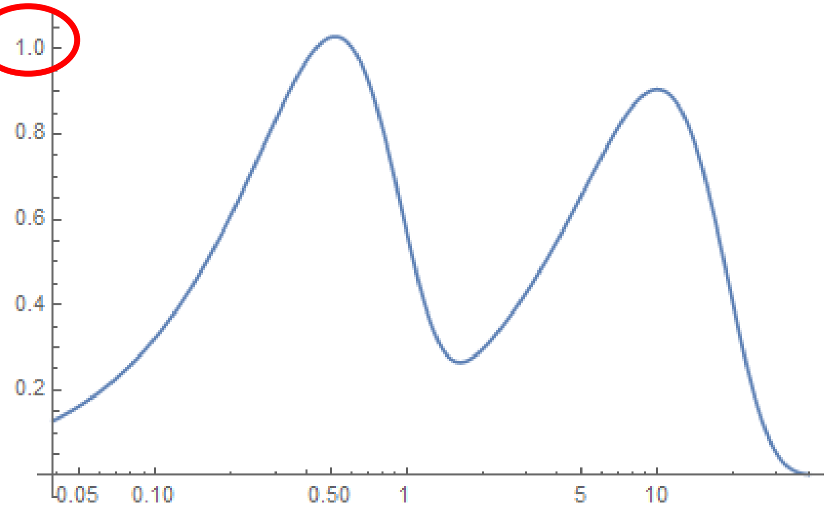
$$f(\boldsymbol{r}_\parallel, t) \equiv \left.\frac{r_\parallel G_s(\boldsymbol{r}_\parallel, t)}{\sigma p_{\mathcal{N}}(\sigma, t|\sigma)}\right|_{\sigma=\sqrt{2\langle D_\parallel\rangle t}}$$

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

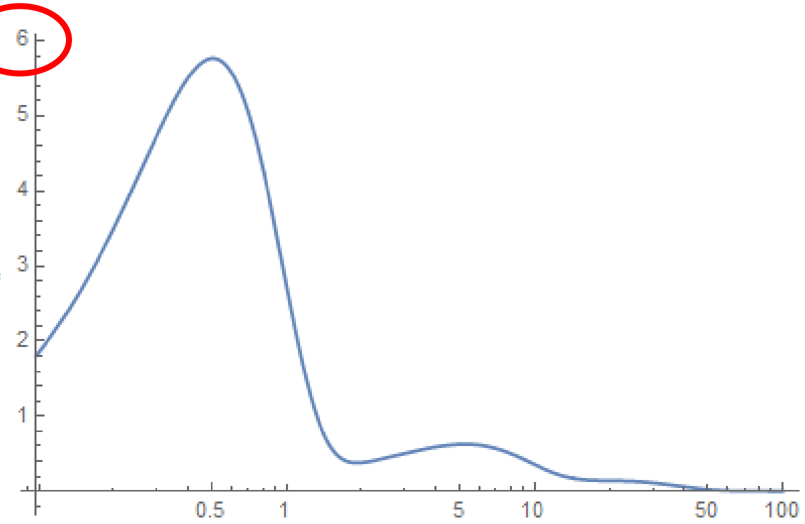
Out[31]=



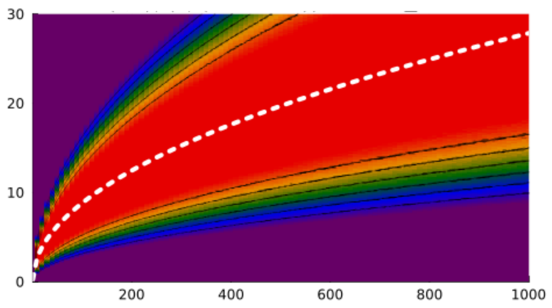
Out[41]=

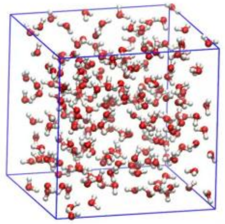


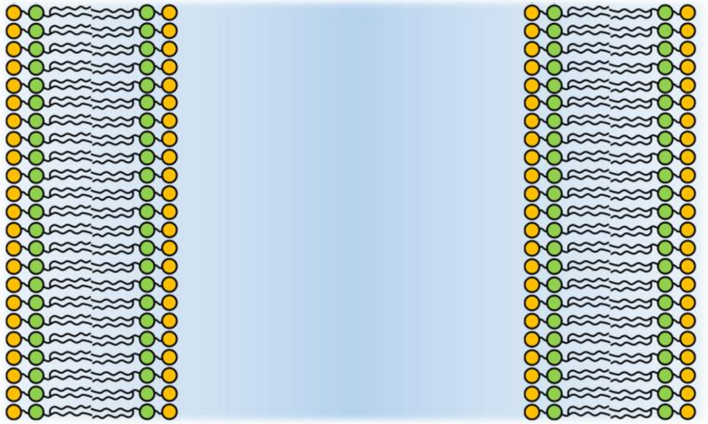
Out[42]=

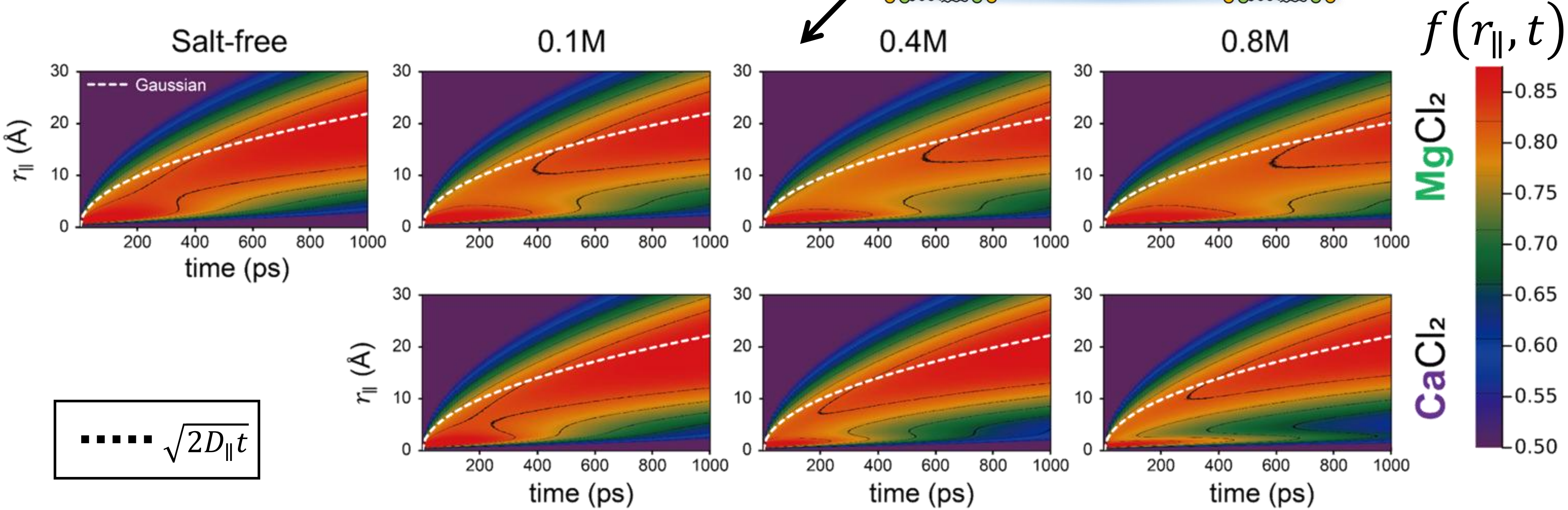


SI Result 1 (c): Lateral Displacement Distribution

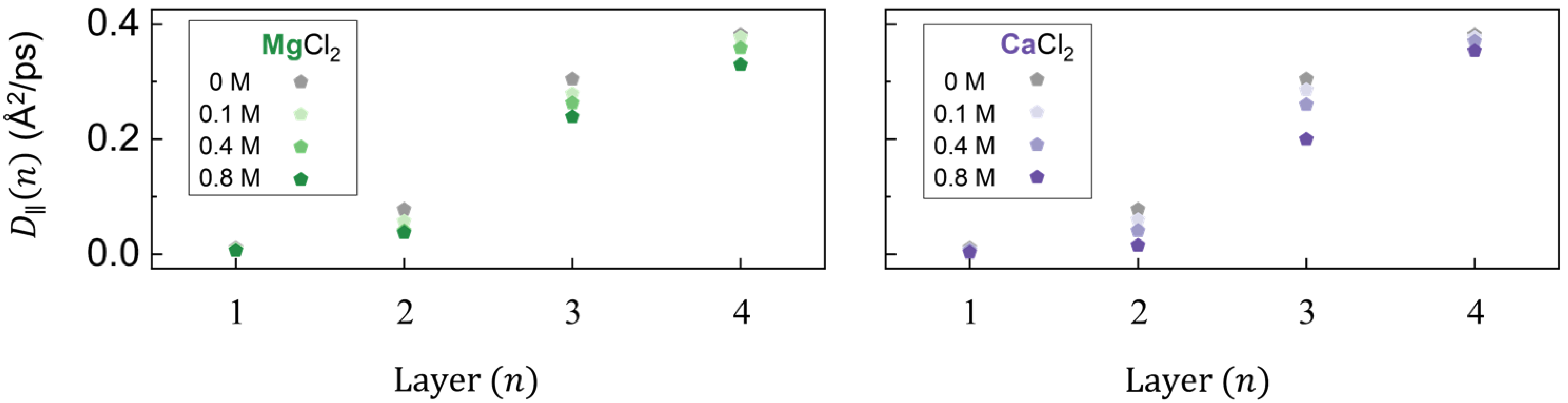








SI Result 1 (d): Region dependent lateral diffusion coefficient

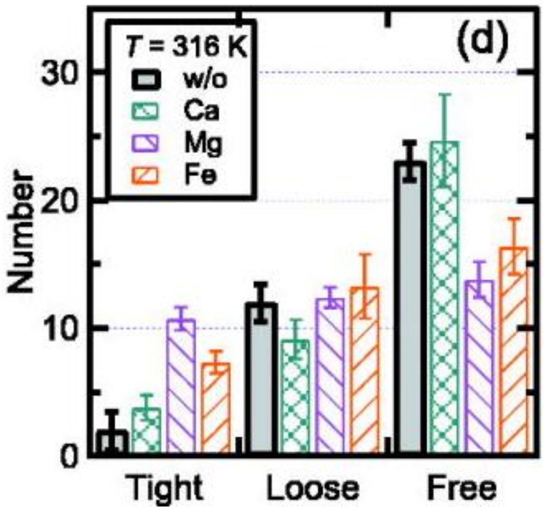


$D_{\parallel}(n)$: determined by umbrella sampling (1 μs-long)

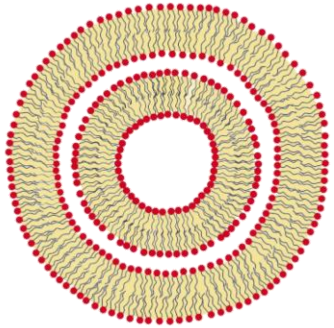
Layer(n): defined by the nodes of $\langle P_2(\cos\theta)\rangle(z)$ in the salt-free case. (see **Fig. 2 (e)**)

SI Result 1 (e): Experimental result

Fig. 3



[Experiment]
DMPC
37 H_2O/lipid molecule.
0.45 M conc.



Multilamellar lipid vesicle

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

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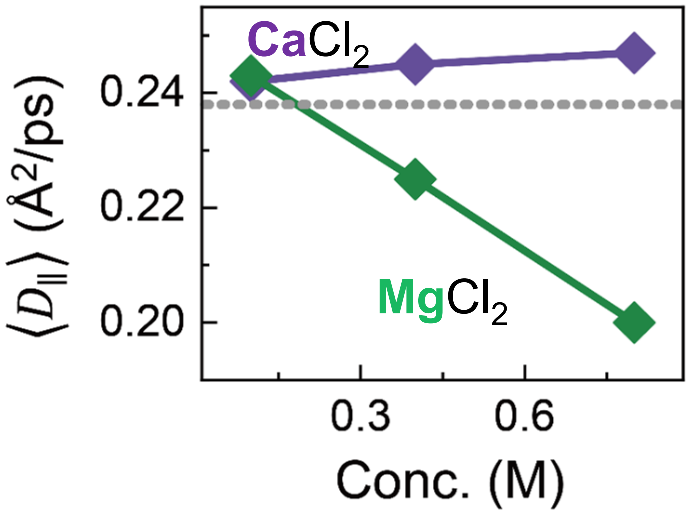
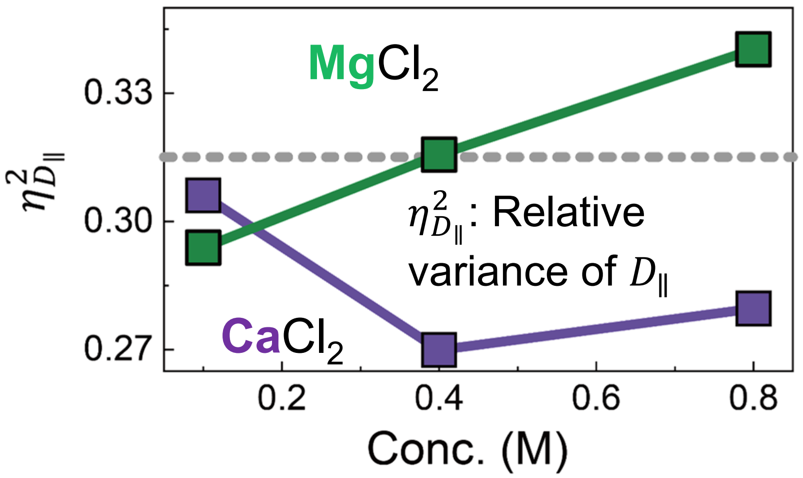
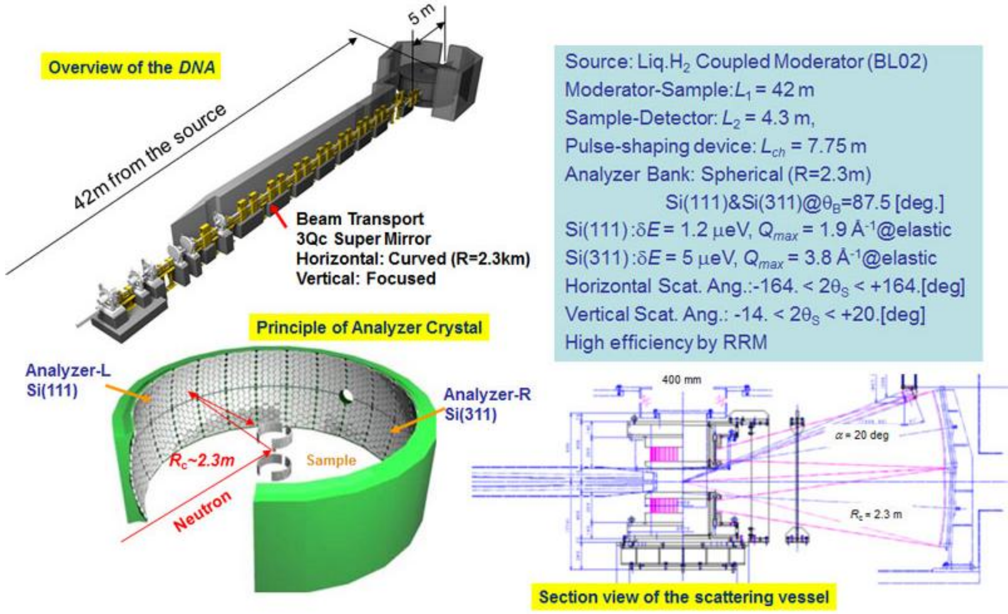


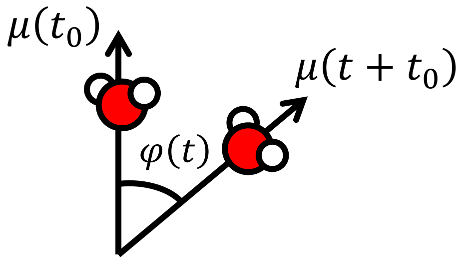


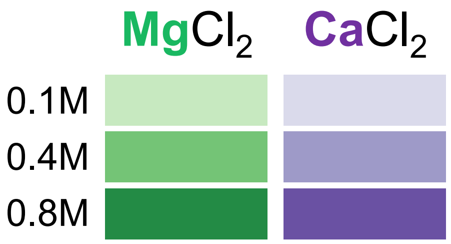


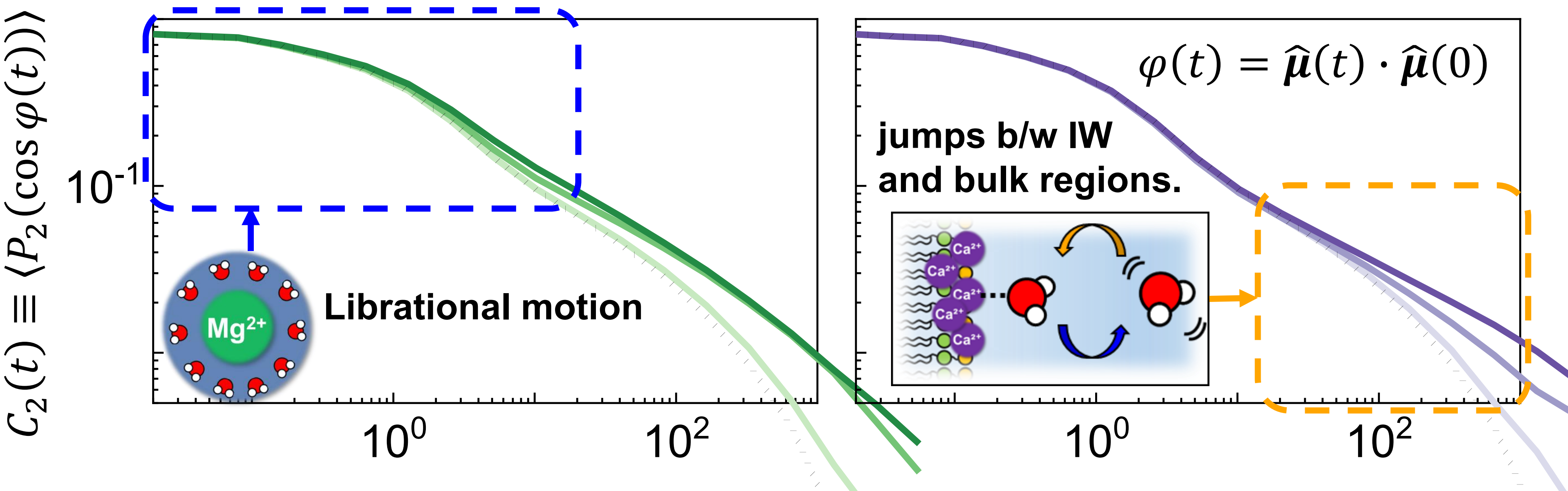
J-PARC MLF BL02 DNA: Dynamic Spectrometer

SI Result 1 (f). Second-order reorientational TCF $C_2(t) \equiv \langle P_2(\cos\varphi(t)) \rangle$

L Bai, *J. Phys. Chem. C.*, 123, 21528-21537 (2019)





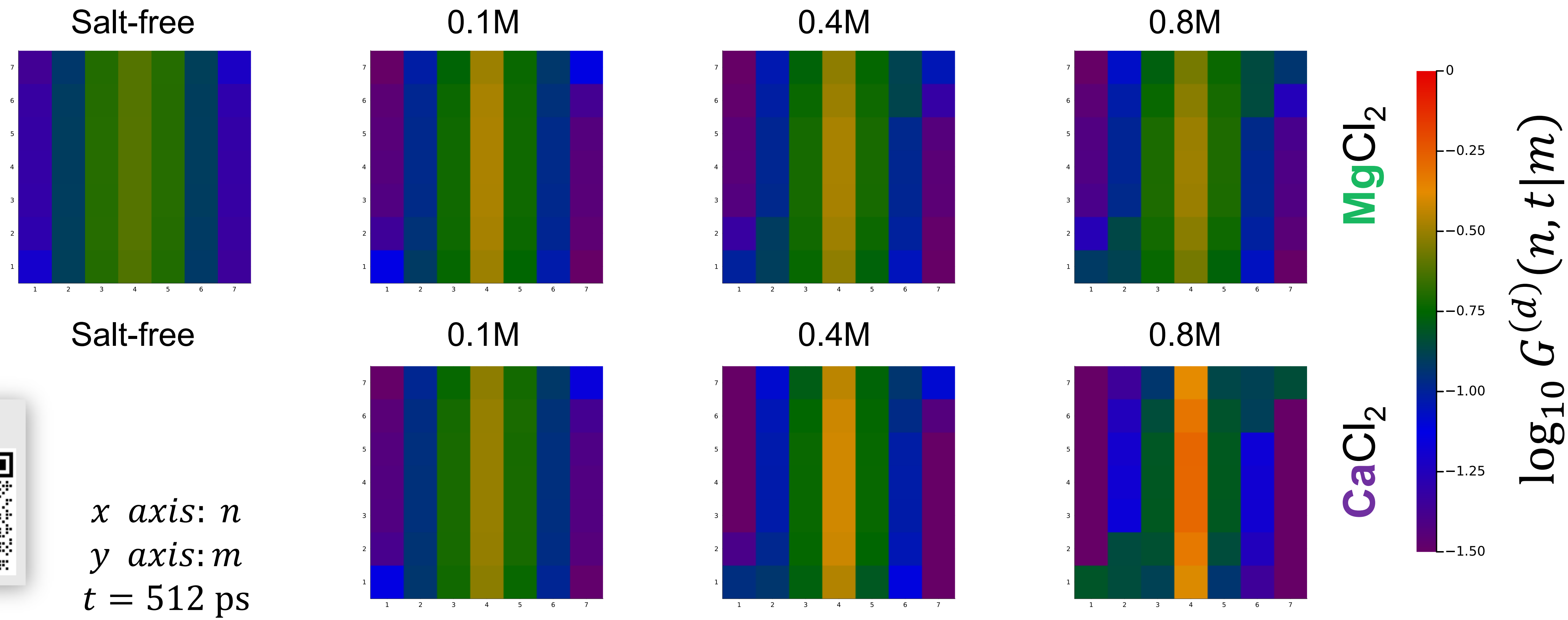


$$\tau_{\text{reor}} \equiv \int_0^\infty dt\, C_2(t)$$

w/o salt
12.57 ps

	0.1M	0.4M	0.8M
$MgCl_2$	15.13 ps	29.50 ps	28.21 ps
$CaCl_2$	14.68 ps	23.35 ps	27.09 ps

SI Result 2. Discrete Green's function $G^{(d)}(n, t|m)$



SI. 2

- The gap between membranes was divided into **7 discrete regions**.
- For sufficiently large t, $G^{(d)}(n, t|m)$ converges to $P_{st}(n)$.
- Higher Conc. leads to a longer timescale for this process. (i.e., $G^{(d)}(n, t|m) \neq P_{st}(n)$) (See **SI Video**)