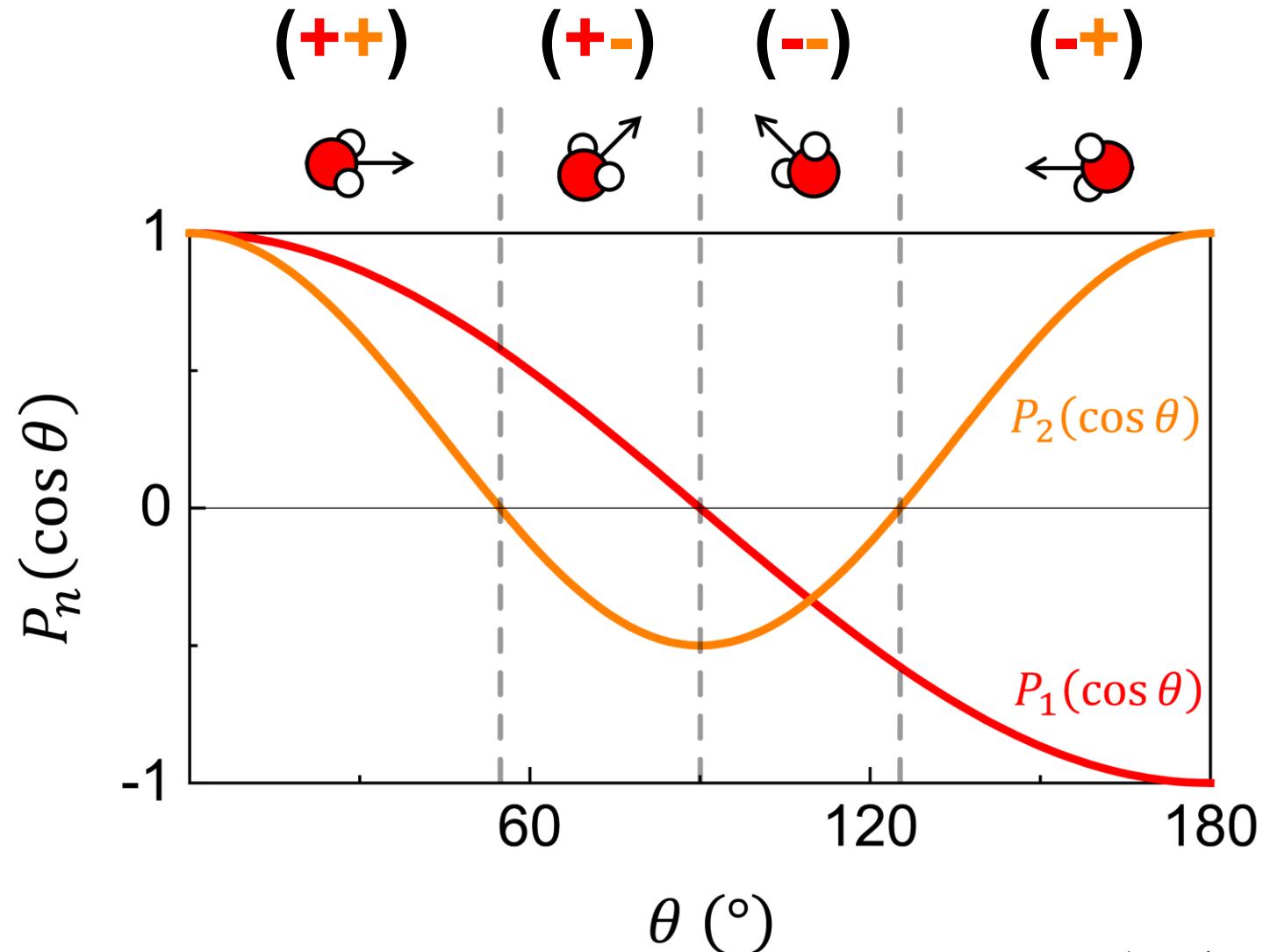


SI Result 1 (a): Legendre Polynomial



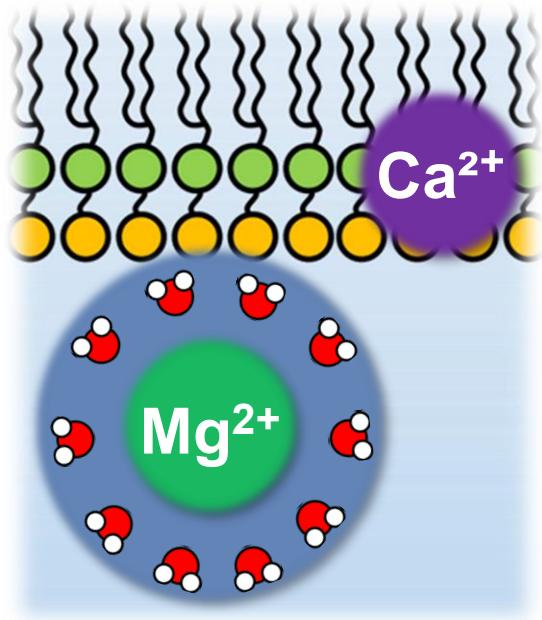
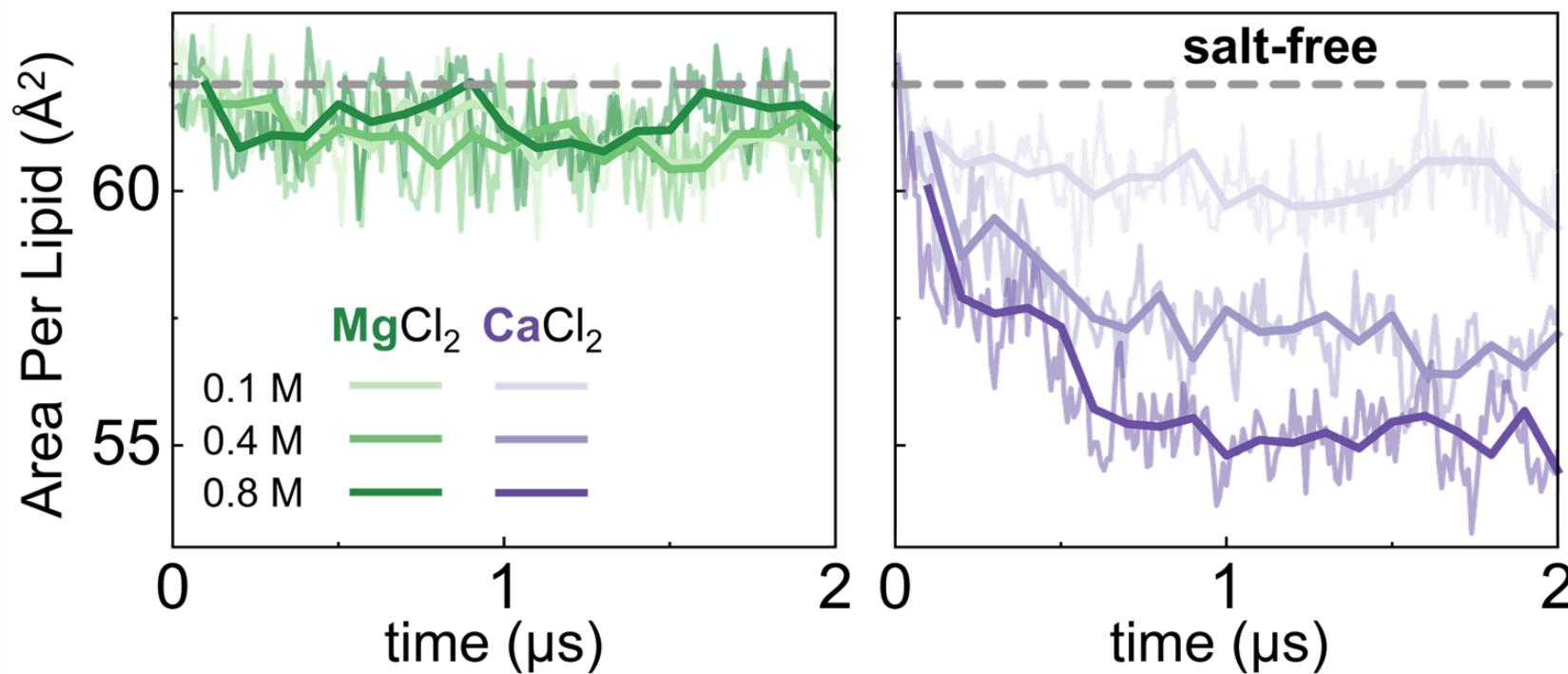
See Fig. 2 (d) and Fig. 2 (e)

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

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

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

SI Result 1 (b): Area per lipid

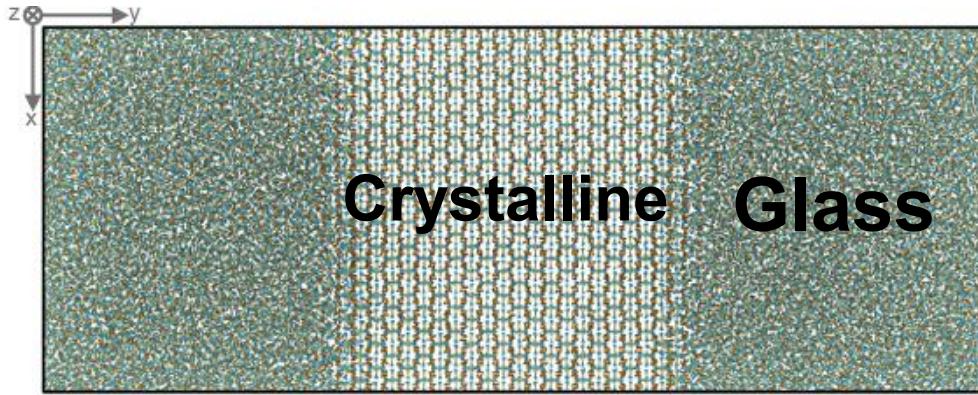


- Mg²⁺ cannot induce membrane condensation due to its **hydration shell** [7].
- Ca²⁺ reduces repulsion between headgroups, inducing **membrane condensation** [7].
- As Conc. of CaCl₂ increases, portion of interfacial water (IW) of CaCl₂ decreases.

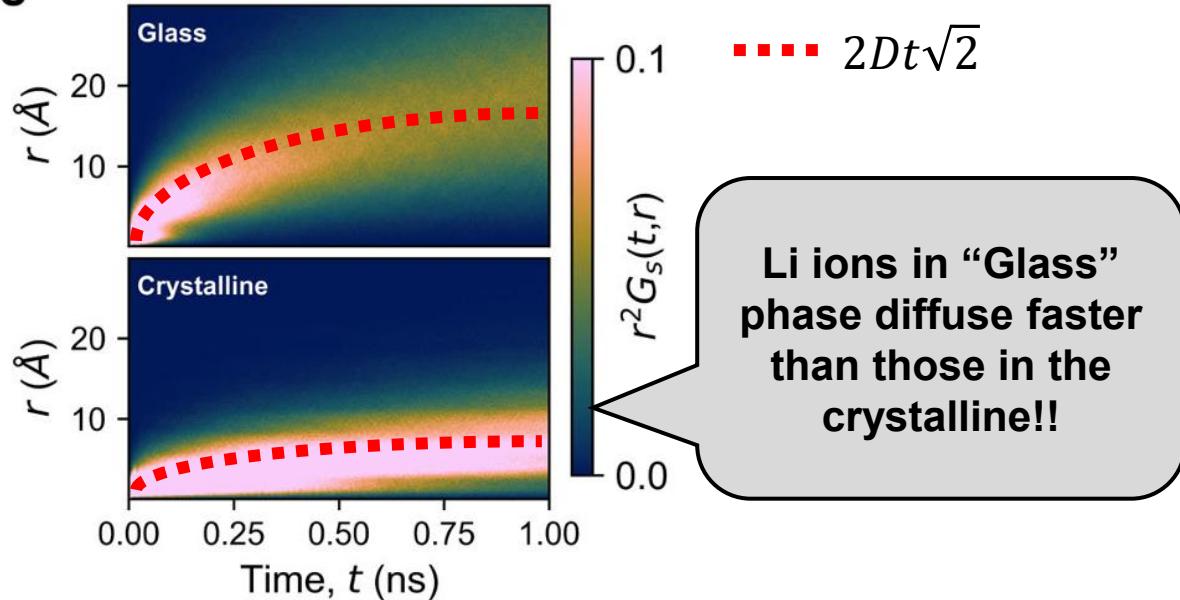
(See $\rho_{H_2O}(z)$ in **Fig. 2 (f)**)

SI Result 1 (c): Lateral Displacement Distribution

Li_3PS_4



C



nature communications



Article

<https://doi.org/10.1038/s41467-025-56322-x>

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

Received: 11 January 2024

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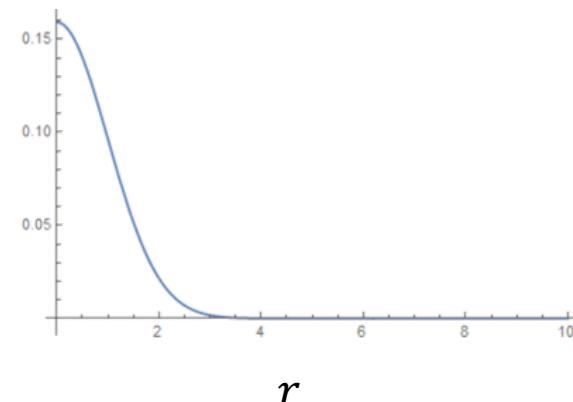
Accepted: 14 January 2025

Morten M. Smedskjaer¹✉

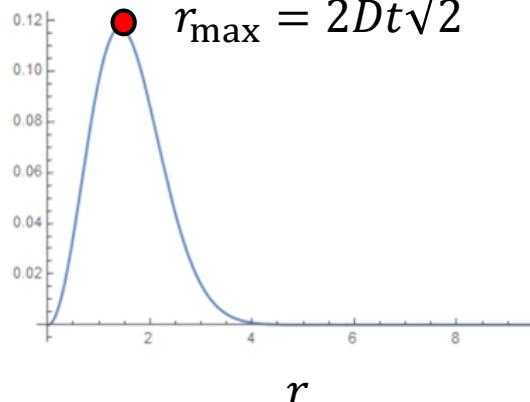
Published online: 26 January 2025

Enhancing the ion conduction in solid electrolytes is critically important for

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



$$r^2 G_s(r, t)$$

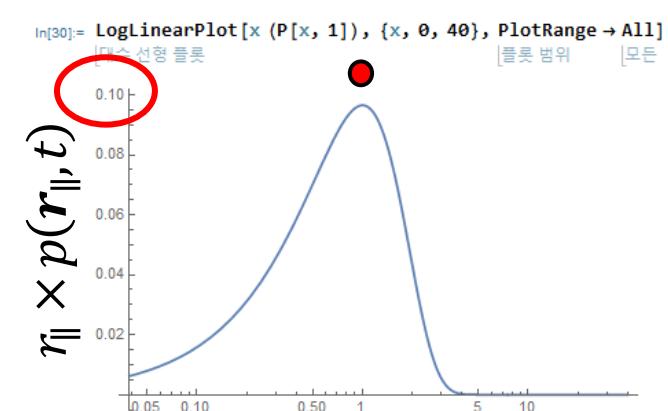


SI Result 1 (c): Lateral Displacement Distribution

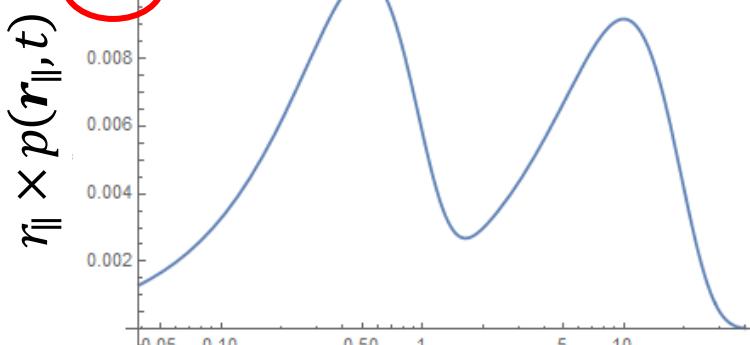
$$G_S(\mathbf{r}_{\parallel}, t) \cong \sum_n f_n G_{\mathcal{N}}(\mathbf{r}_{\parallel}, t | D_{\parallel}^{(n)}) \quad \sum_n f_n = 1 \quad G_{\mathcal{N}}(\mathbf{r}_{\parallel}, t | D_{\parallel}) \equiv (4\pi D_{\parallel} t)^{-1} e^{-r_{\parallel}^2 / 4D_{\parallel} t}$$

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

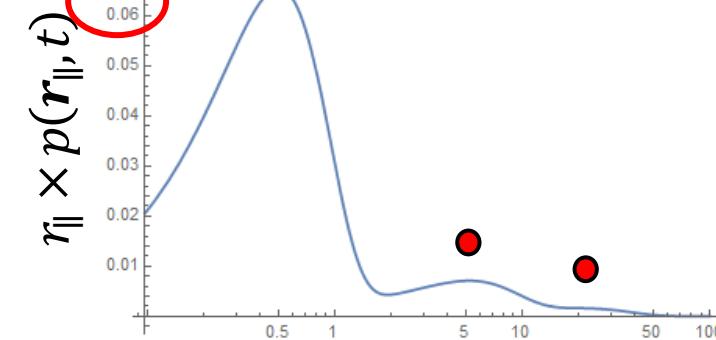
```
In[2]:= P[x_, σ_] := (2 π σ²)^⁻¹ Exp[-x² / (2 σ²)]
```



```
In[28]:= LogLinearPlot[x (0.05 P[x, 0.5] + 0.95 P[x, 10]), {x, 0, 40}, PlotRange -> All]
```



```
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]
```

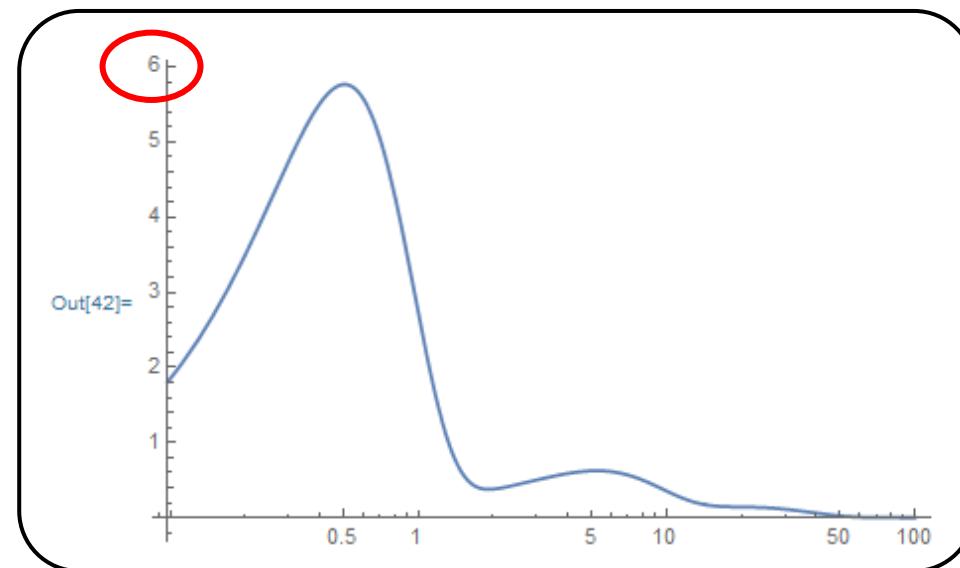
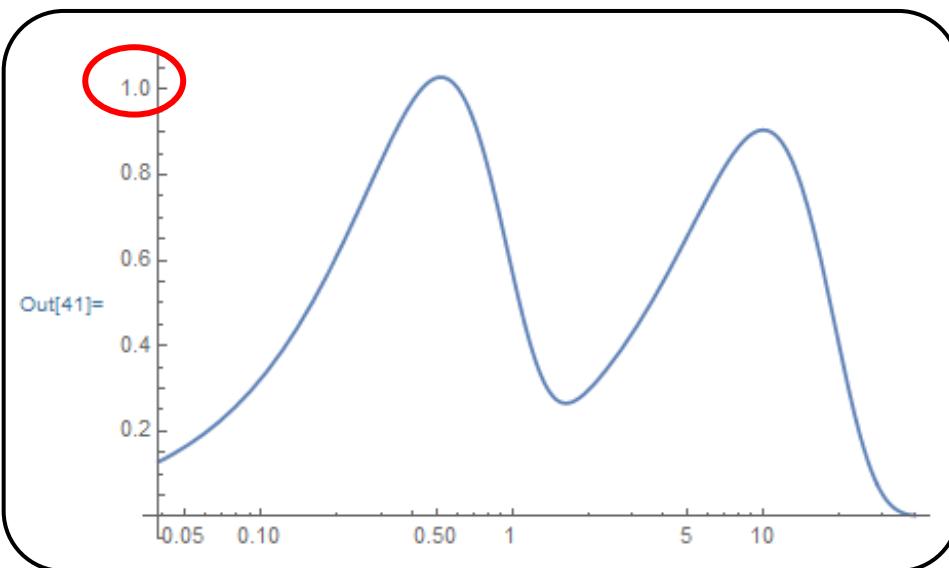
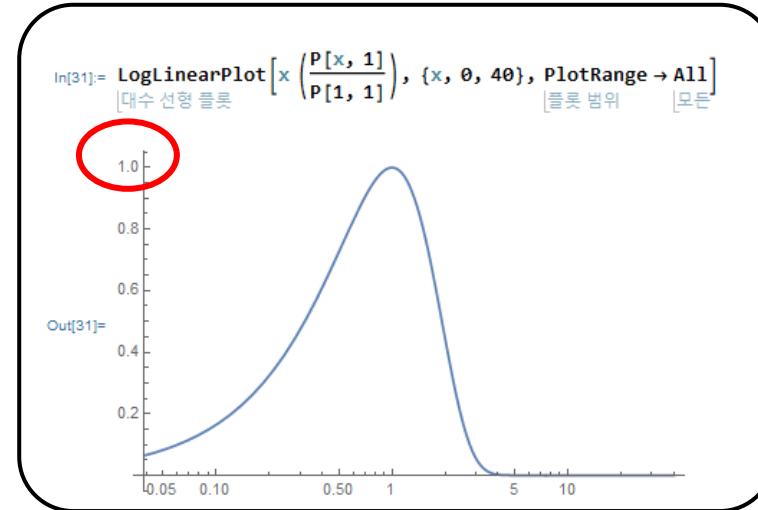


SI Result 1 (c): Lateral Displacement Distribution

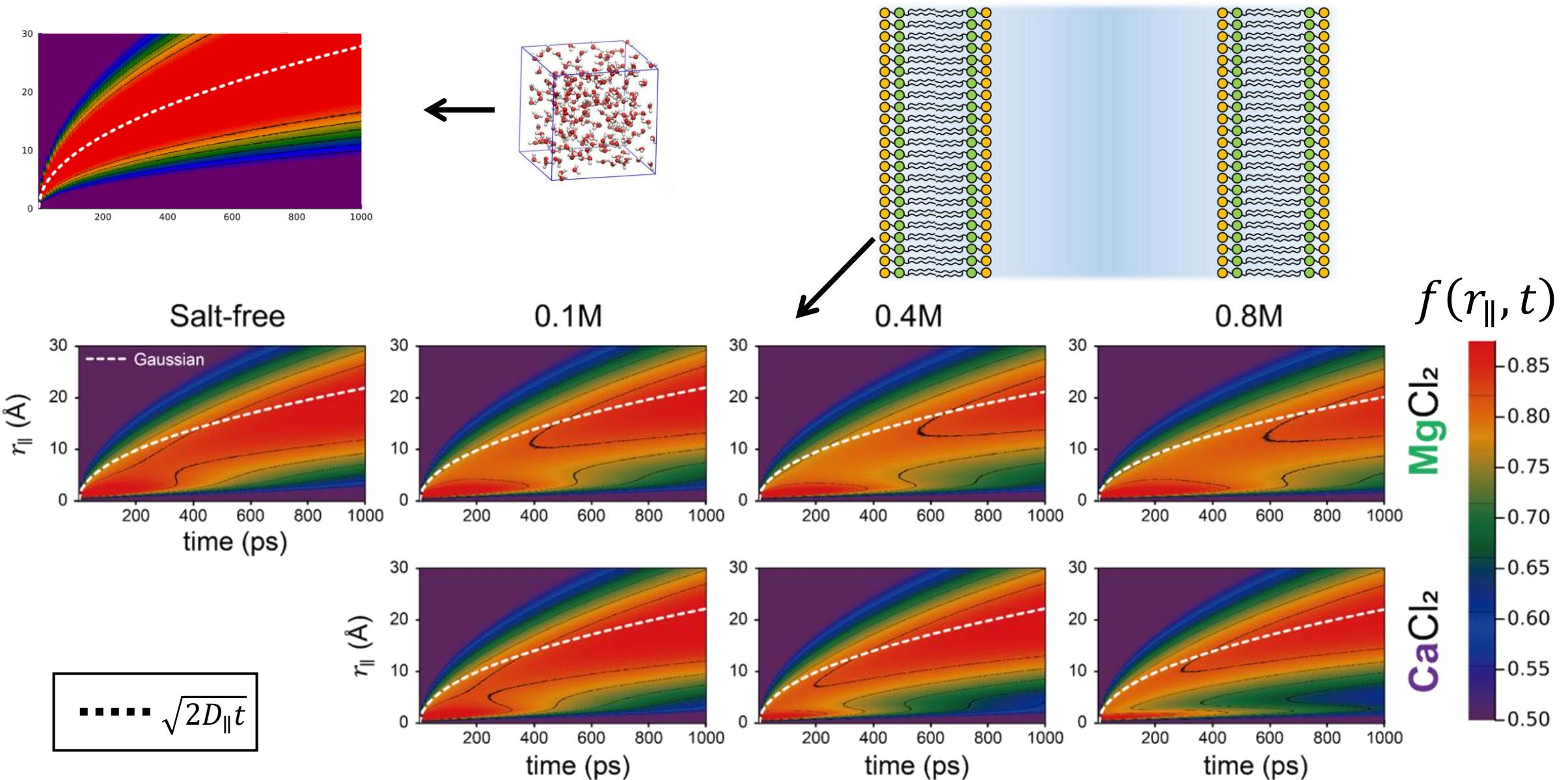
$$G_S(\mathbf{r}_{\parallel}, t) \cong \sum_n f_n G_{\mathcal{N}}(\mathbf{r}_{\parallel}, t | D_{\parallel}^{(n)}) \quad \sum_n f_n = 1$$

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

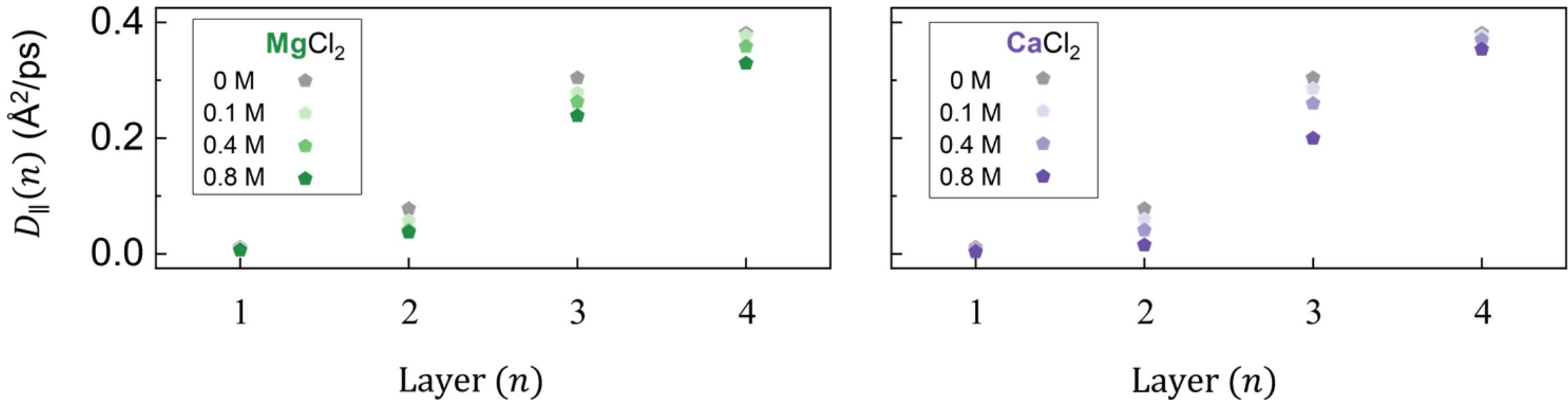
$$f(\mathbf{r}_{\parallel}, t) \equiv \frac{r_{\parallel} G_S(\mathbf{r}_{\parallel}, t)}{\sigma p_{\mathcal{N}}(\sigma, t | \sigma)} \Big|_{\sigma=\sqrt{2\langle D_{\parallel} \rangle t}}$$



SI Result 1 (c): Lateral Displacement Distribution



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

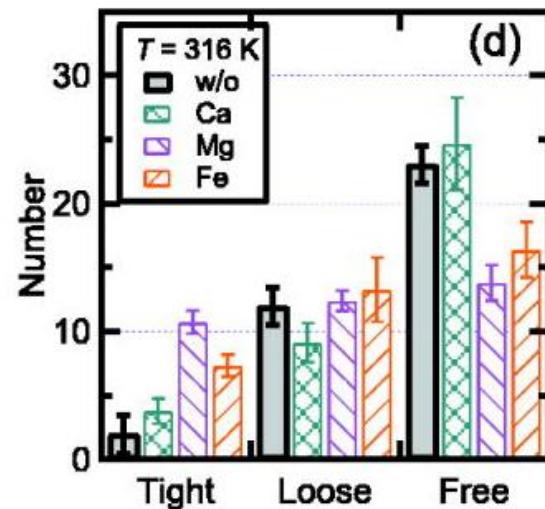


$D_{\parallel}(n)$: determined by umbrella sampling (1 μs -long)

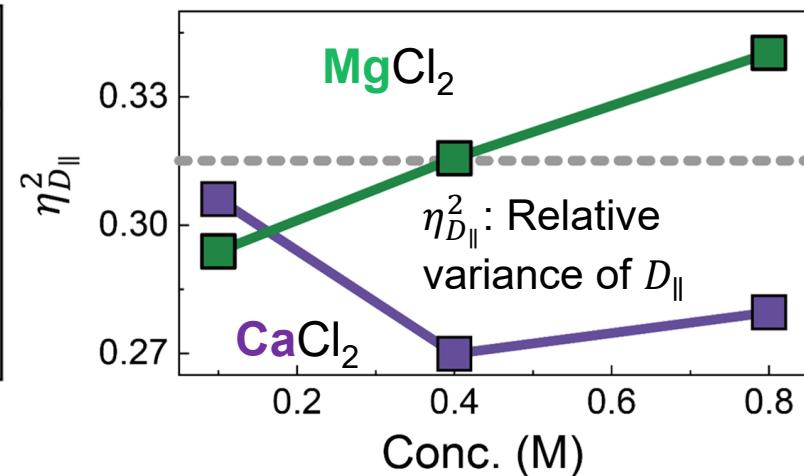
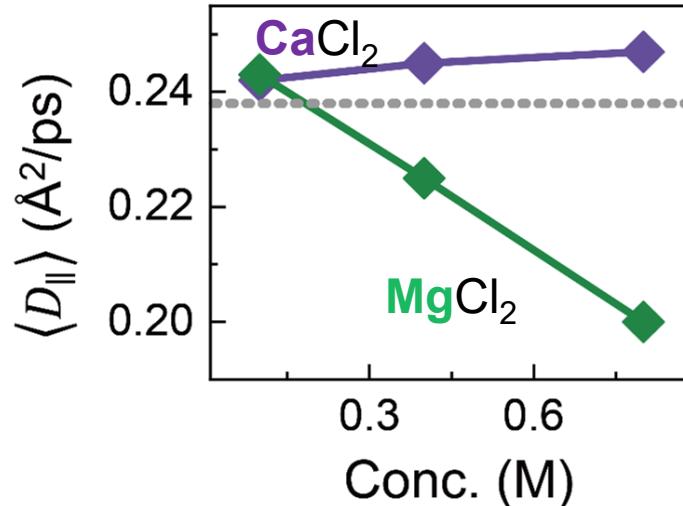
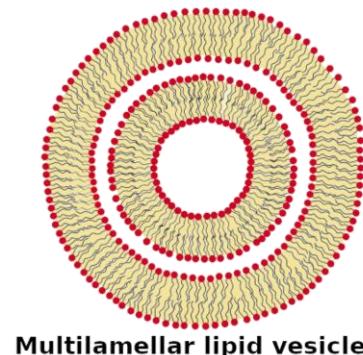
Layer(n): defined by the nodes of $\langle P_2(\cos \theta) \rangle(z)$ in the salt-free case. (see Fig. 2 (e))

SI Result 1 (e): Experimental result

Fig. 3



[Experiment]
DMPC
37 $\text{H}_2\text{O}/\text{lipid molecule}$.
0.45 M conc.



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

Cite as: Appl. Phys. Lett. **116**, 133701 (2020); doi:10.1063/1.5144012
Submitted: 31 December 2019 · Accepted: 26 February 2020 ·
Published Online: 30 March 2020

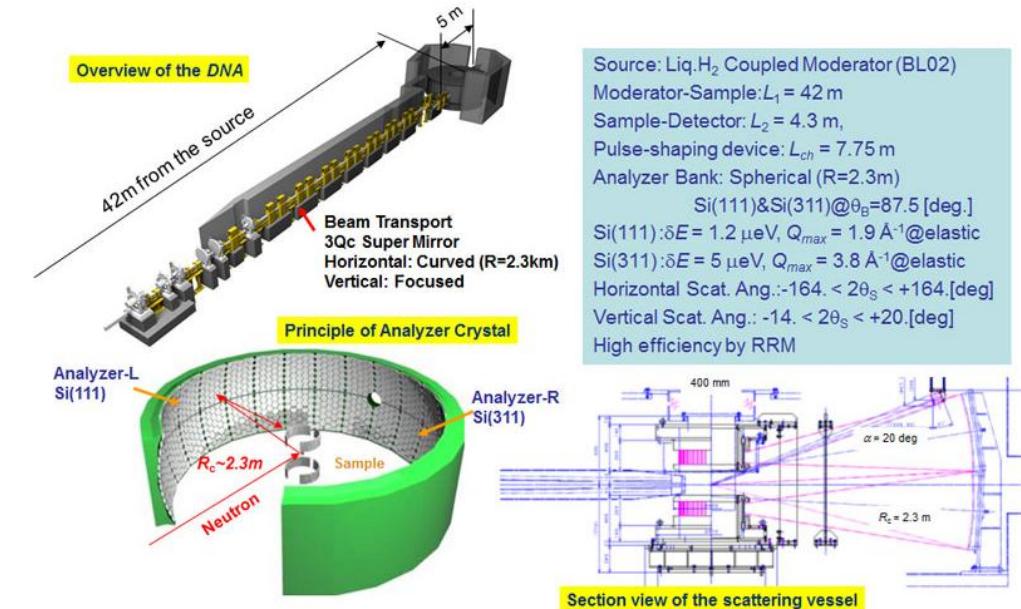
H. Seto^{1,a)} and T. Yamada^{2,b)}

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²Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, Tokai 319-1106, Japan

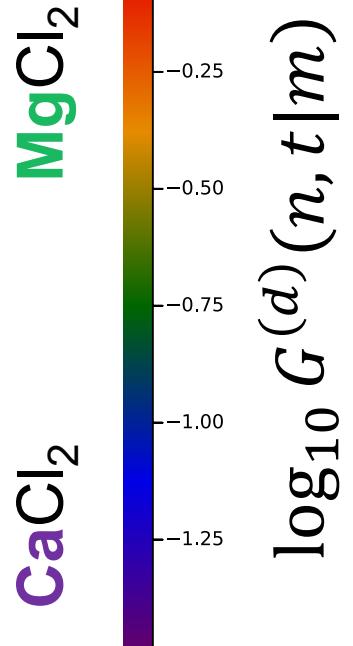
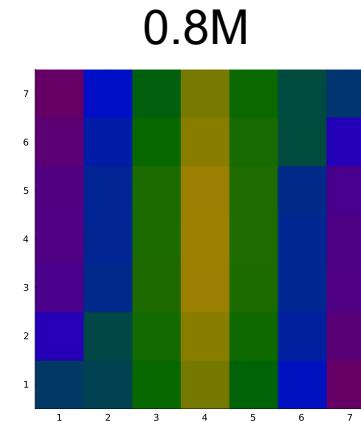
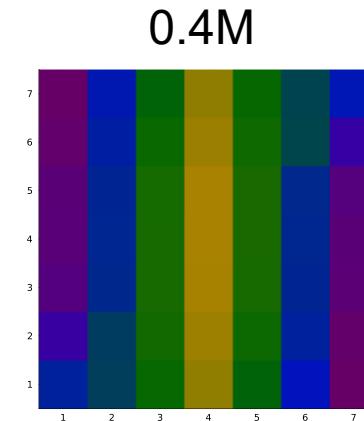
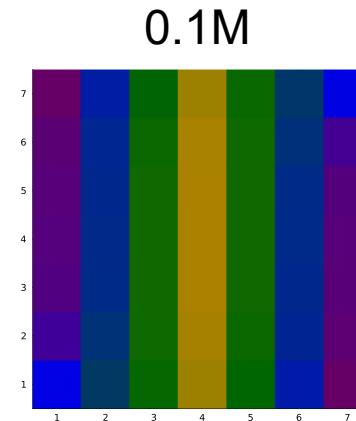
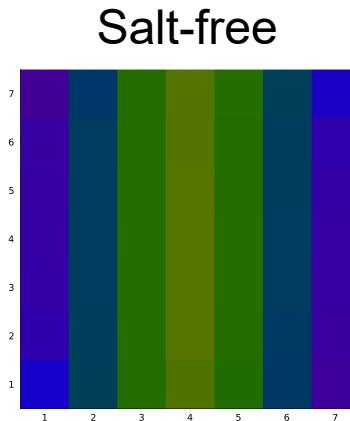
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J-PARC MLF BL02 DNA: Dynamic Spectrometer

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



Salt-free

0.1M

0.4M

0.8M

SI. 2



x axis: n
 y axis: m
 $t = 512$ ps

- 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**)