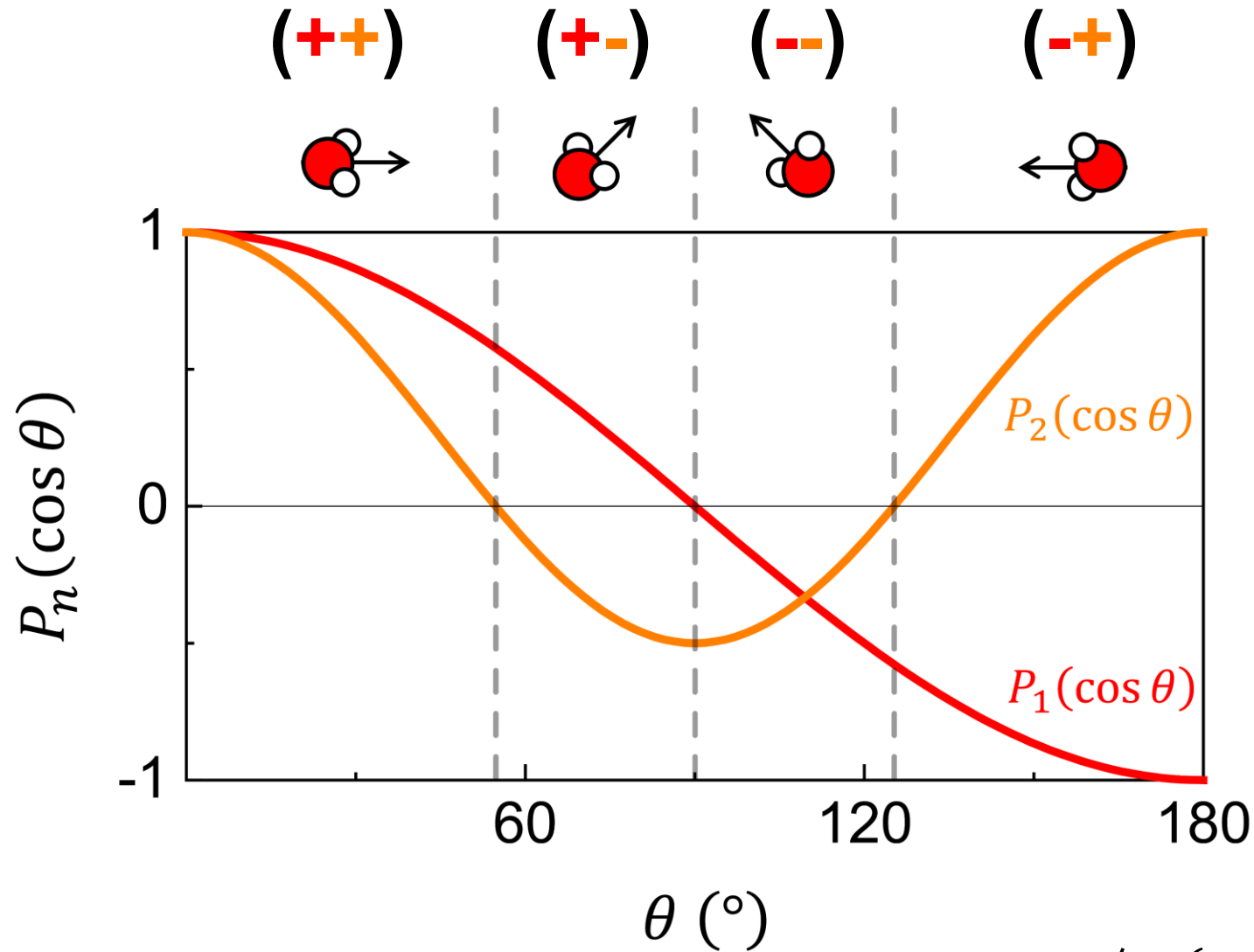


SI Result 1 (a): Legendre Polynomial



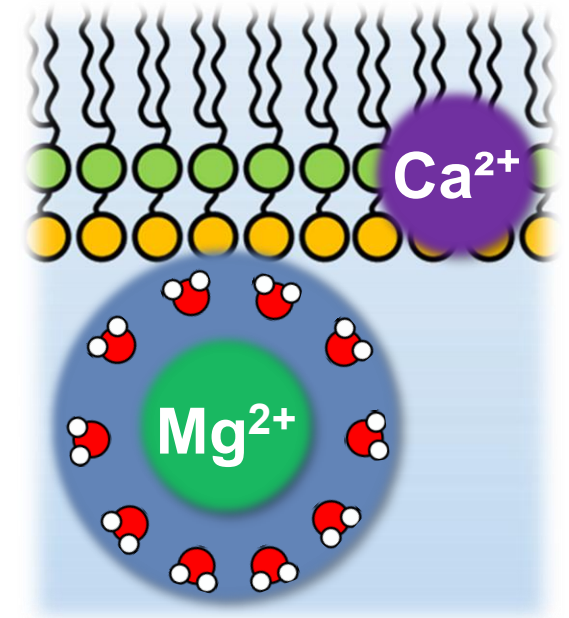
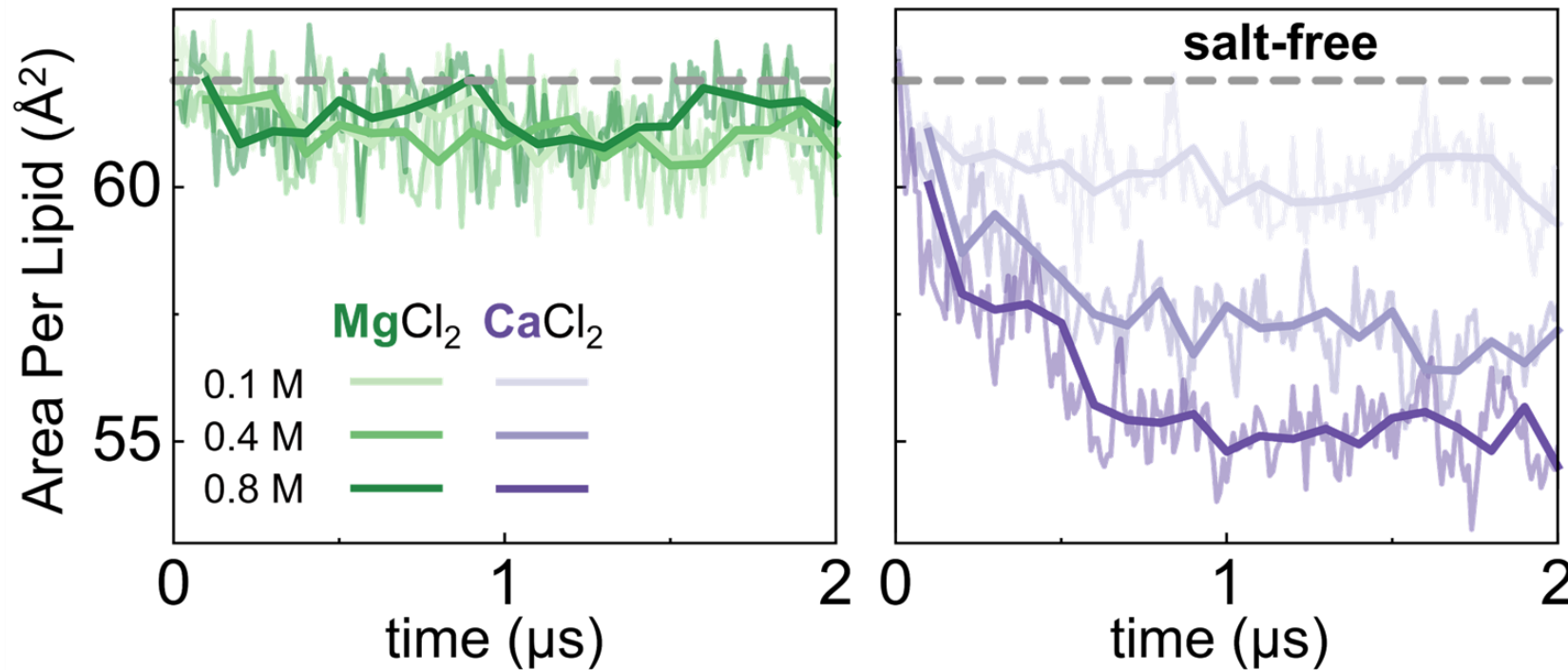
See **Fig. 2 (d)** and **Fig. 2 (e)**

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

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

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

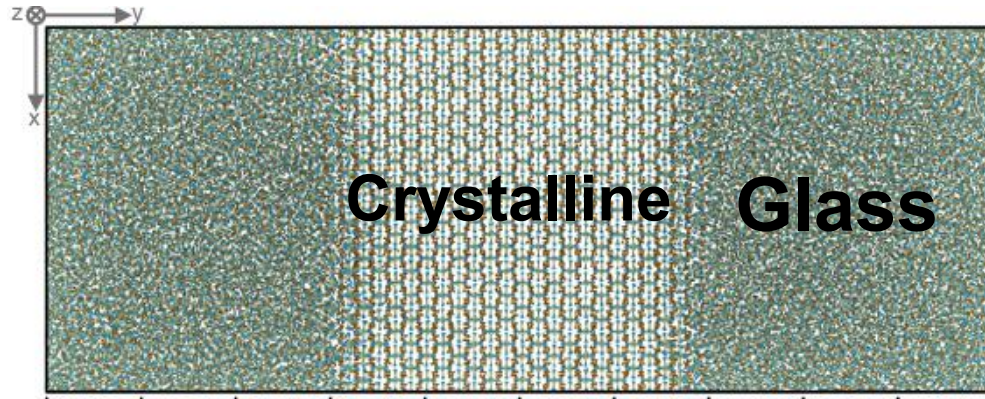
SI Result 1 (b): Area per lipid



- 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)**)

SI Result 1 (c): Lateral Displacement Distribution



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

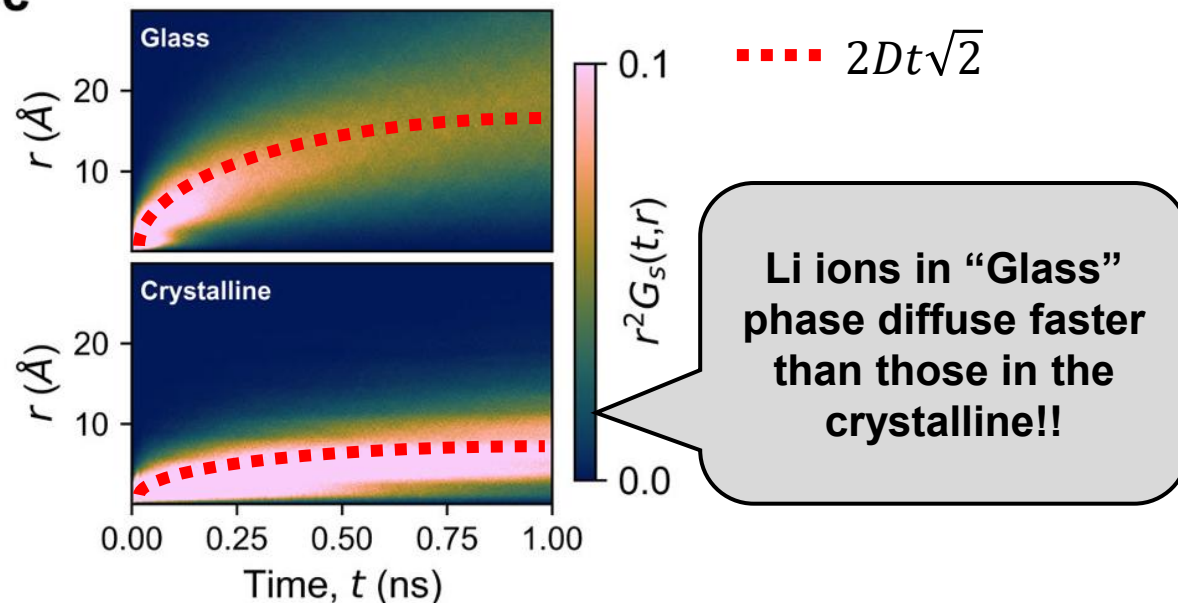
Zhimin Chen¹, Tao Du^{1,2}✉, N. M. Anoop Krishnan³, Yuanzheng Yue¹ & Morten M. Smedskjaer¹✉

Accepted: 14 January 2025

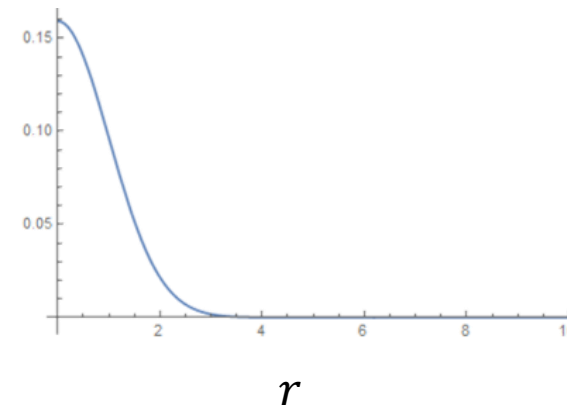
Published online: 26 January 2025

Enhancing the ion conduction in solid electrolytes is critically important for

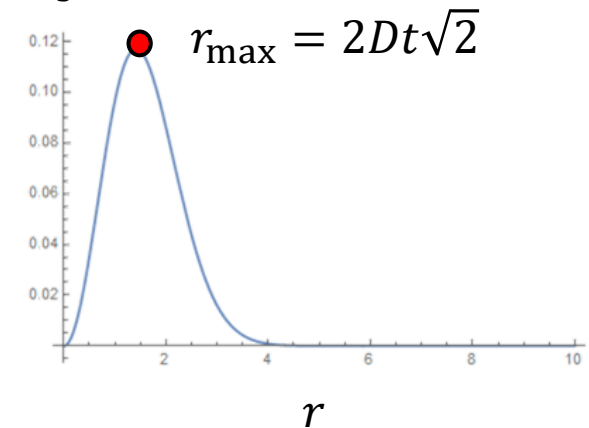
c



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



$$r^2 G_S(\mathbf{r}, t)$$



SI Result 1 (c): Lateral Displacement Distribution

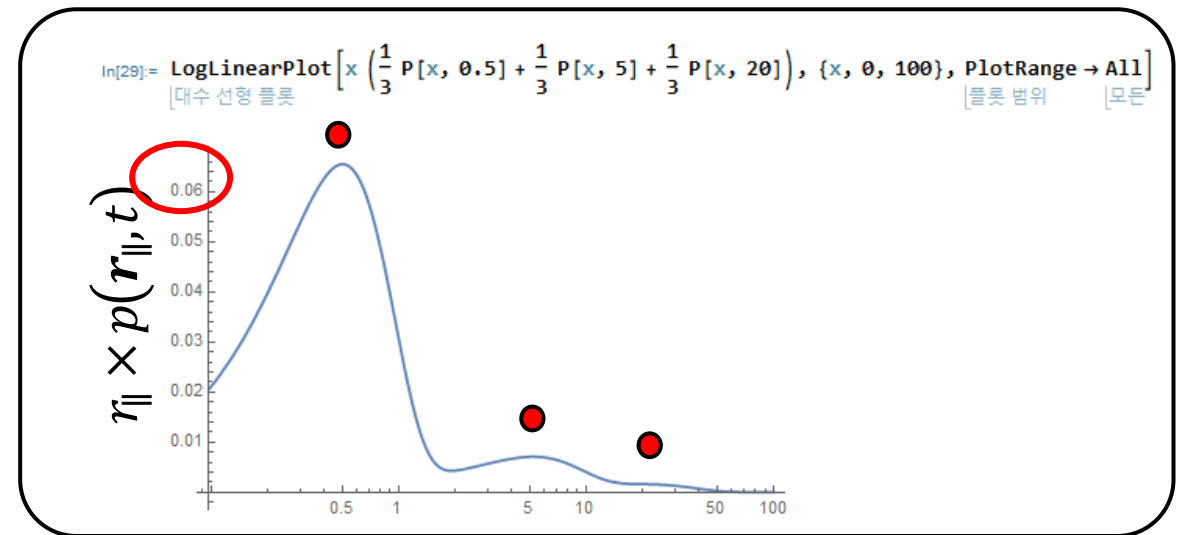
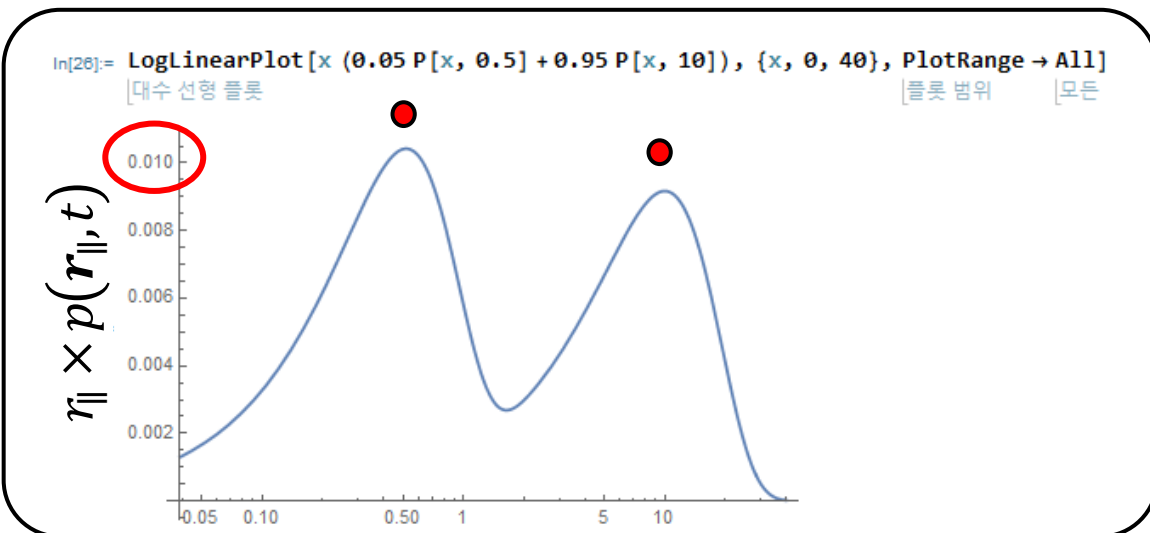
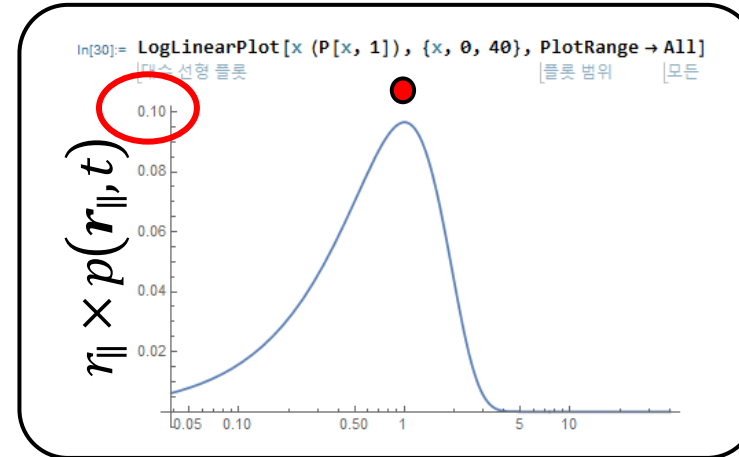
$$G_S(\mathbf{r}_{\parallel}, t) \cong \sum_n f_n G_N(\mathbf{r}_{\parallel}, t | D_{\parallel}^{(n)}) \quad \sum_n f_n = 1$$

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

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

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

[지수 함수]

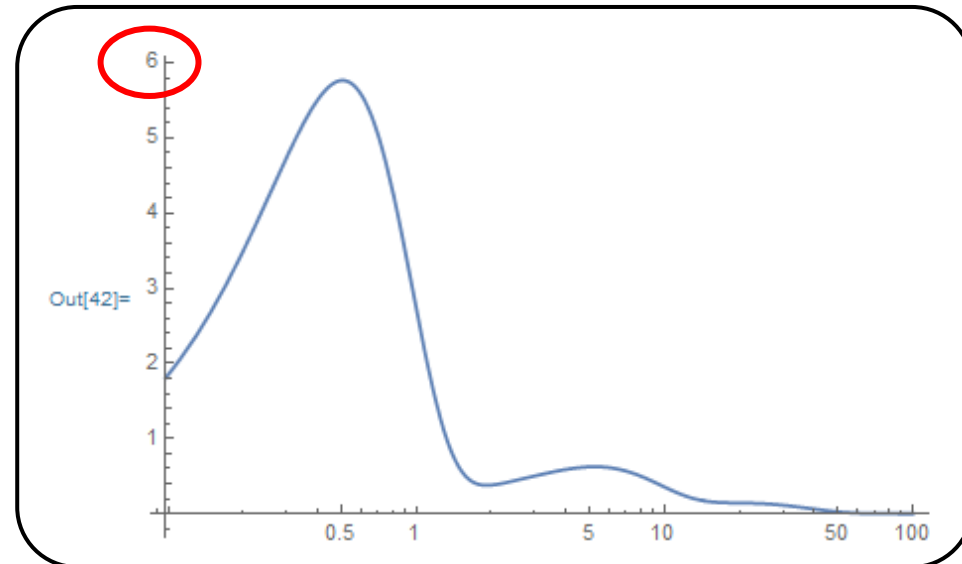
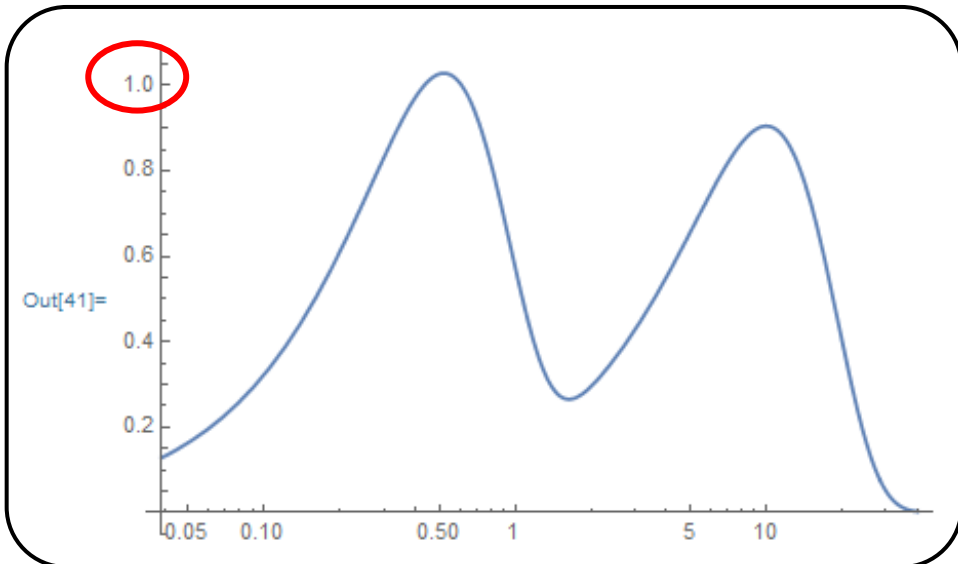
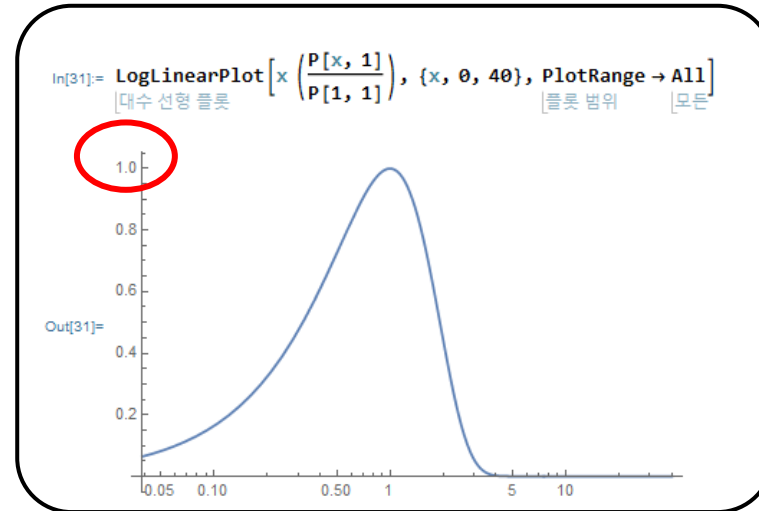


SI Result 1 (c): Lateral Displacement Distribution

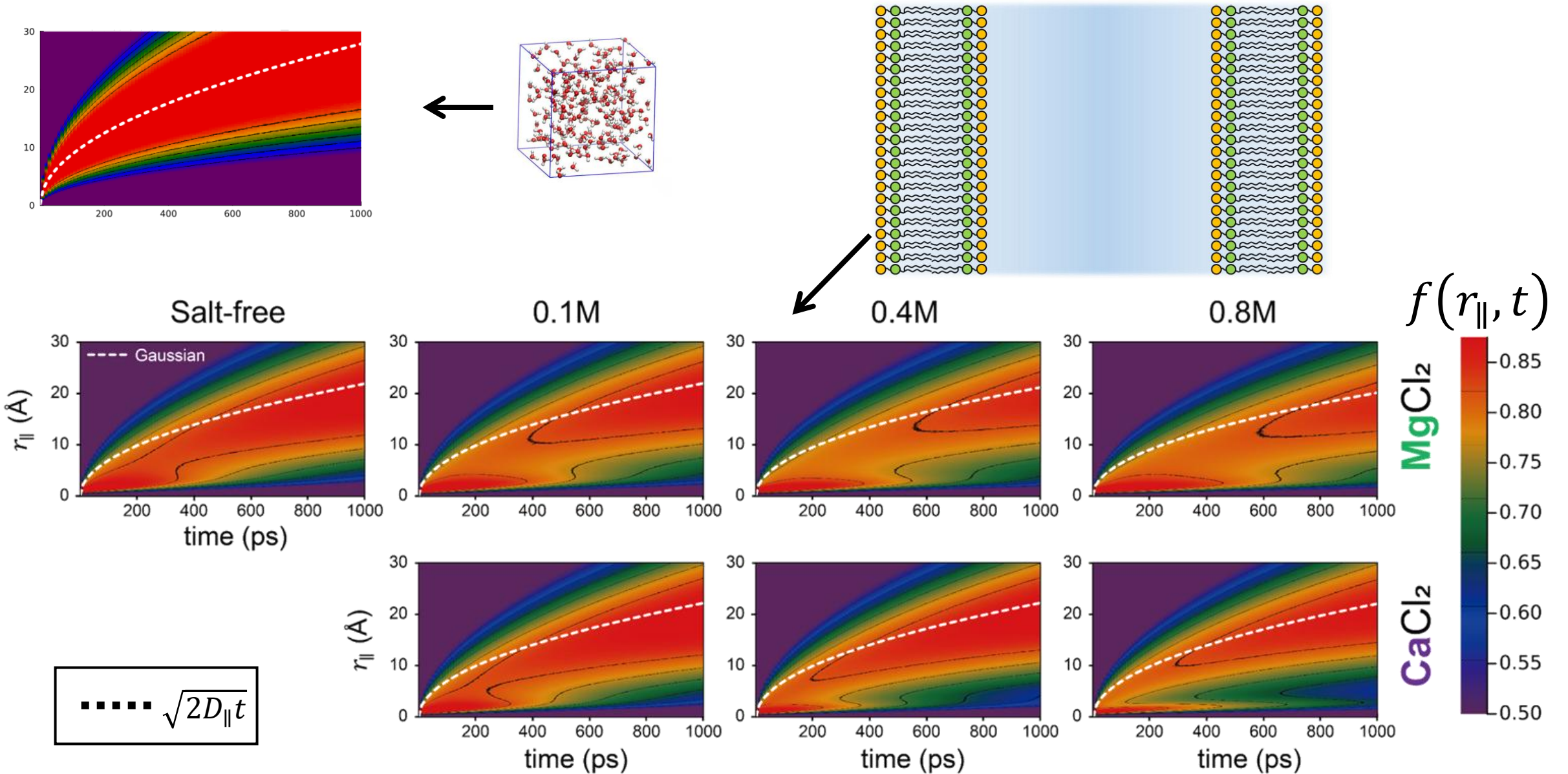
$$G_s(\mathbf{r}_{\parallel}, t) \cong \sum_n f_n G_{\mathcal{N}}(\mathbf{r}_{\parallel}, t | D_{\parallel}^{(n)}) \quad \sum_n f_n = 1$$

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

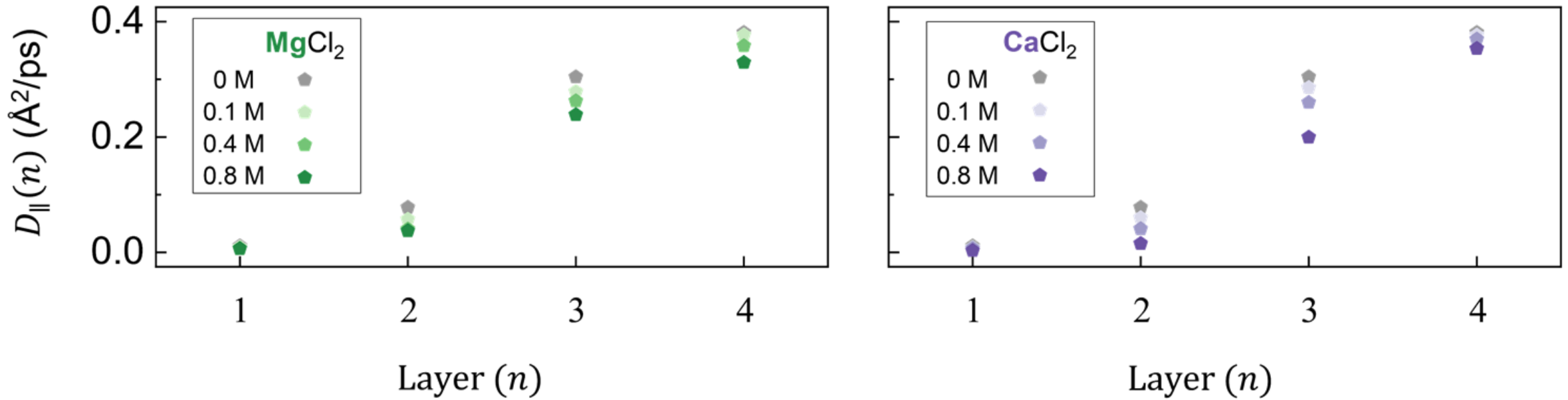
$$G_{\mathcal{N}}(\mathbf{r}_{\parallel}, t | D_{\parallel}) \equiv (4\pi D_{\parallel} t)^{-1} e^{-r_{\parallel}^2 / 4 D_{\parallel} t}$$



SI Result 1 (c): Lateral Displacement Distribution



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

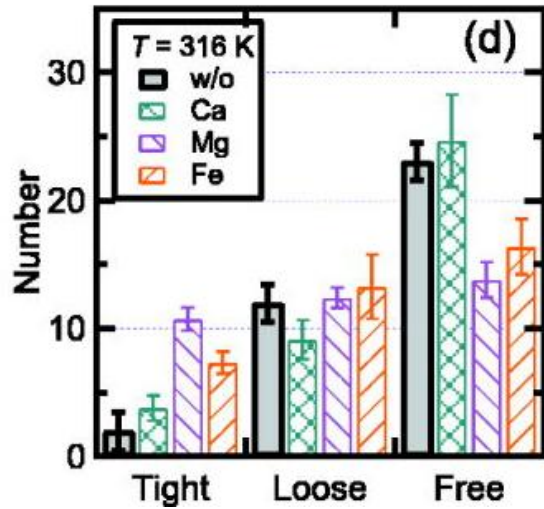


$D_{\parallel}(n)$: determined by umbrella sampling (1 μs -long)

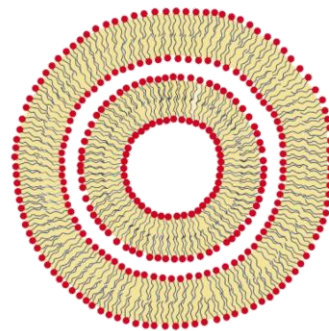
Layer(n): defined by the nodes of $\langle P_2(\cos \theta) \rangle(z)$ in the salt-free case. (see **Fig. 2 (e)**)

SI Result 1 (e): Experimental result

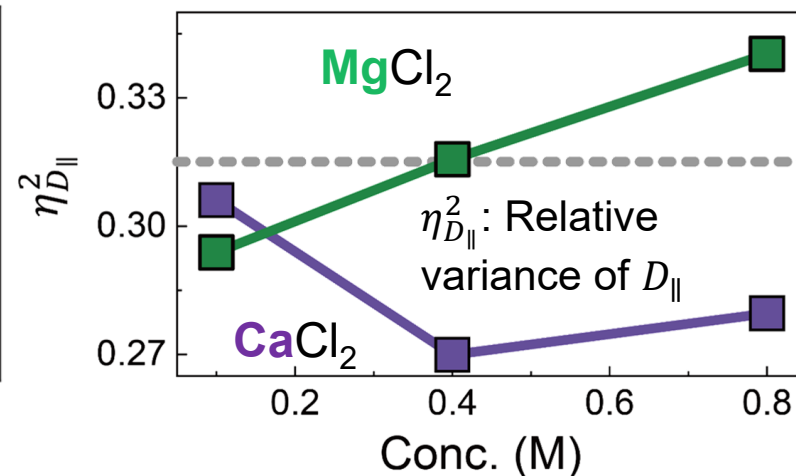
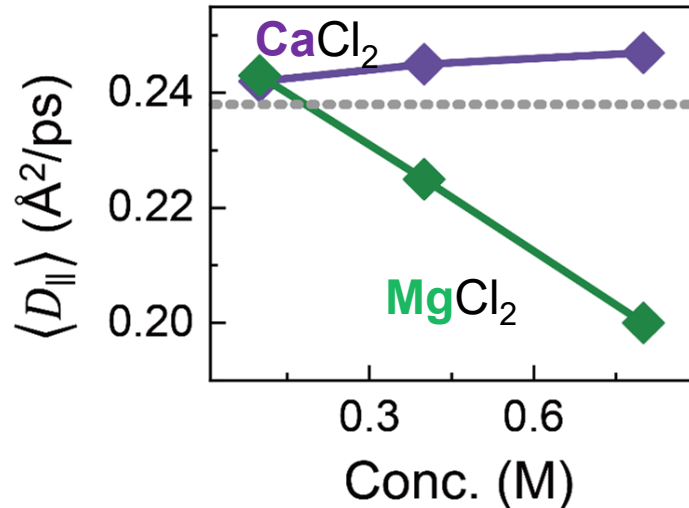
Fig. 3



[Experiment]
DMPC
37 H₂O/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

Cite as: Appl. Phys. Lett. **116**, 133701 (2020); doi: [10.1063/1.5144012](https://doi.org/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)}

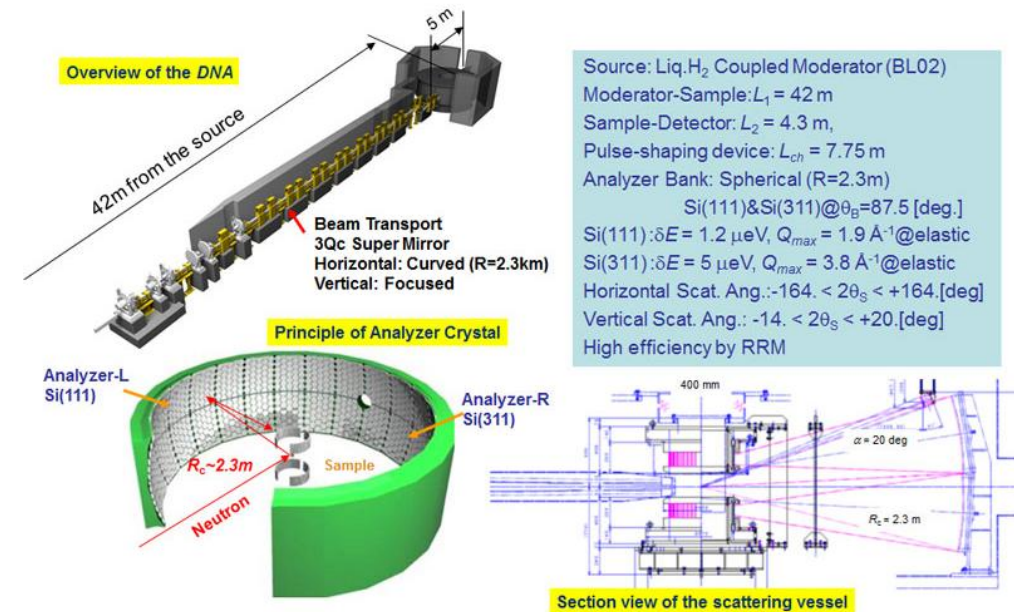
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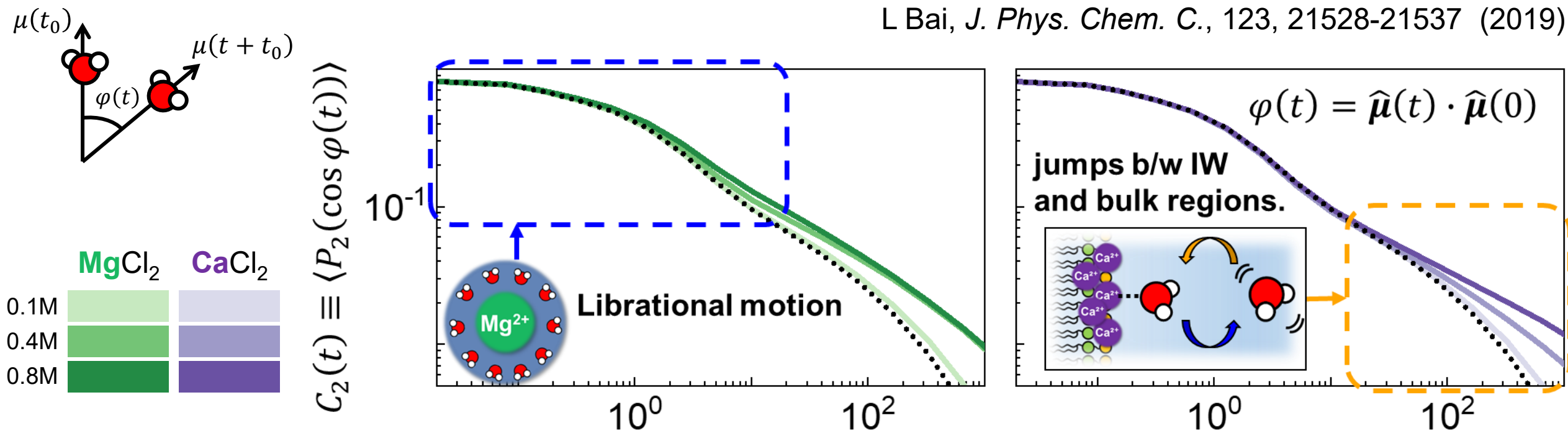
^{b)}Electronic mail: t.yamada@cross.or.jp



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)

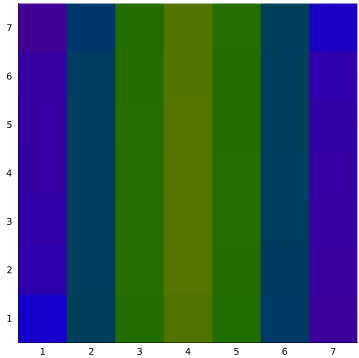


$$\tau_{\text{reor}} \equiv \int_0^\infty dt C_2(t)$$

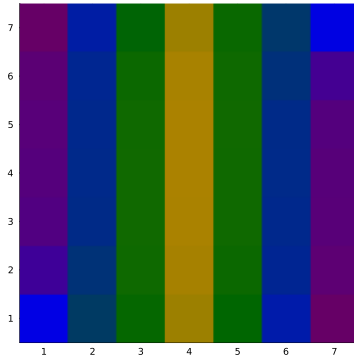
	0 M	0.1M	0.4M	0.8M
MgCl ₂	12.57 ps	15.13 ps	29.50 ps	28.21 ps
CaCl ₂	12.57 ps	14.68 ps	23.35 ps	27.09 ps

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

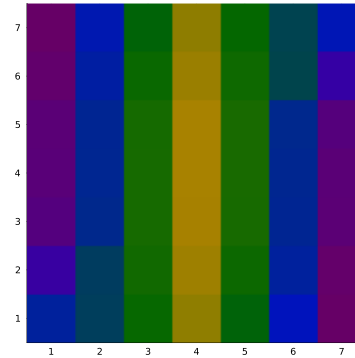
Salt-free



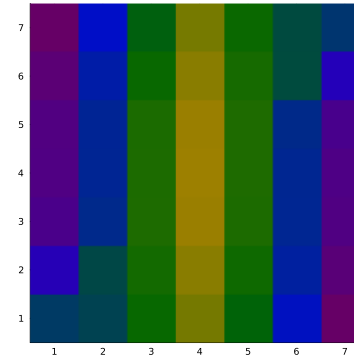
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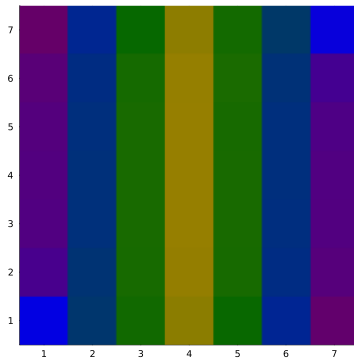
0.4M



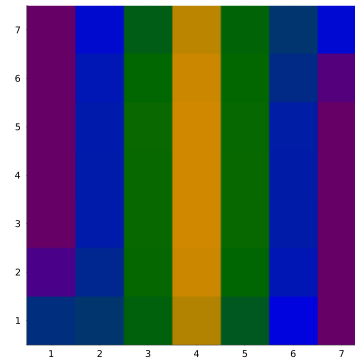
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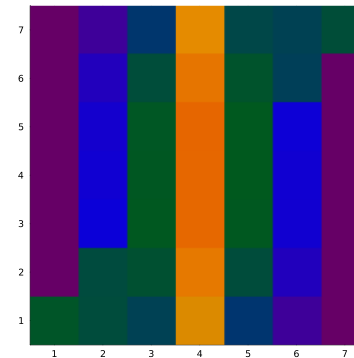
Salt-free



0.1M



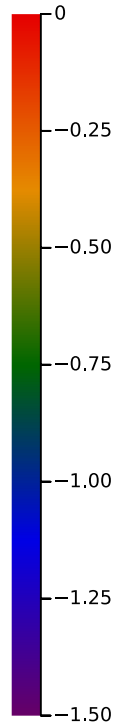
0.4M



0.8M

MgCl_2

CaCl_2



$\log_{10} G^{(d)}(n, t|m)$

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**)