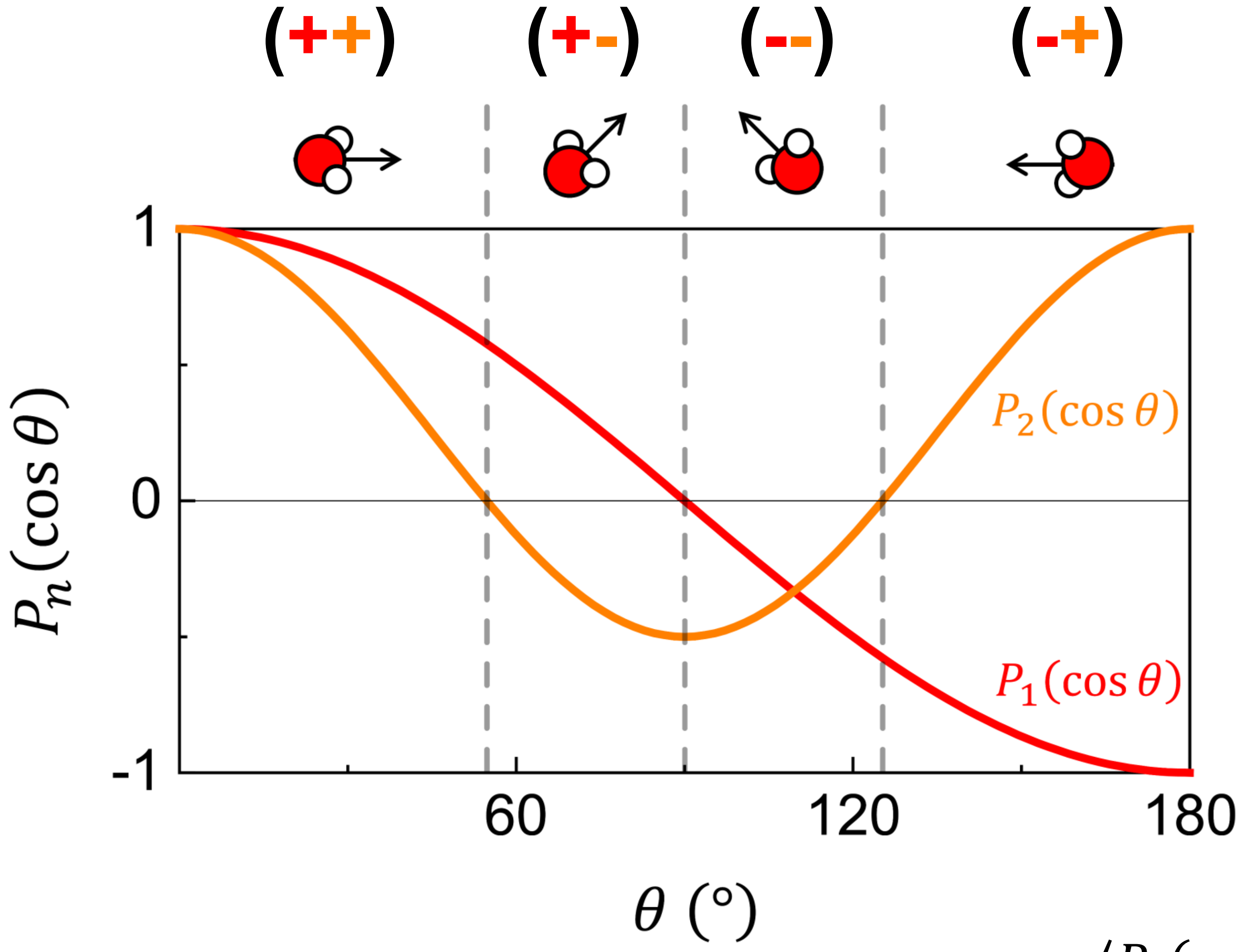
SI Result 1 (a): Legendre Polynomial



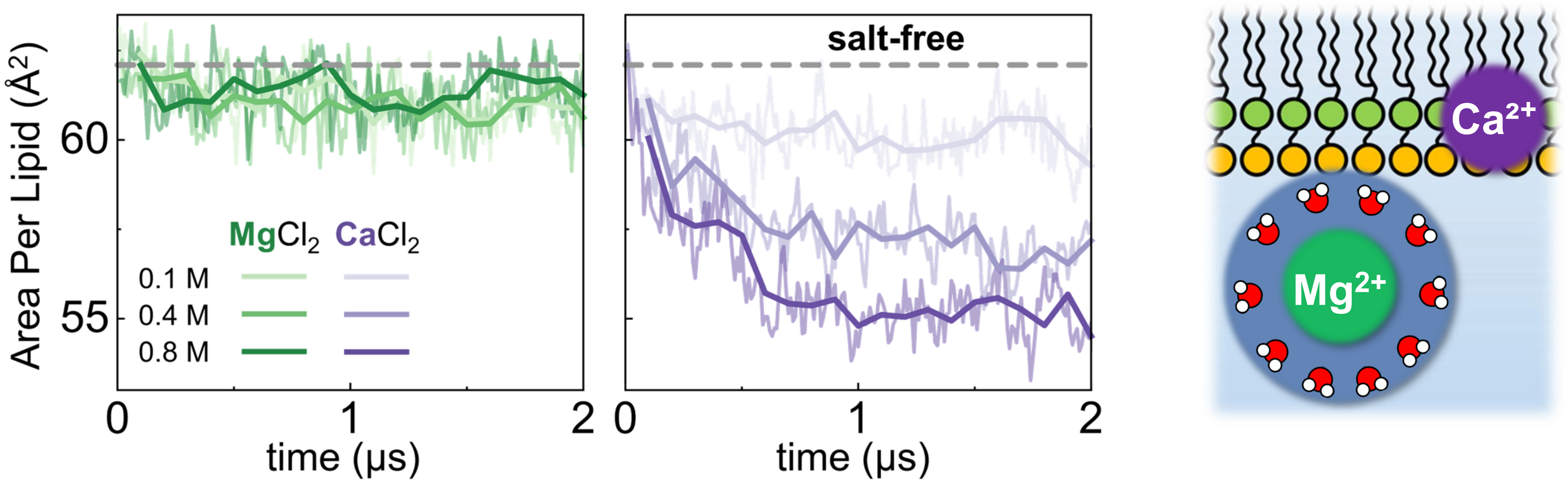
See **Fig. 2 (d)** and **Fig. 2 (e)**

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

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

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

SI Result 1 (b): Area per lipid



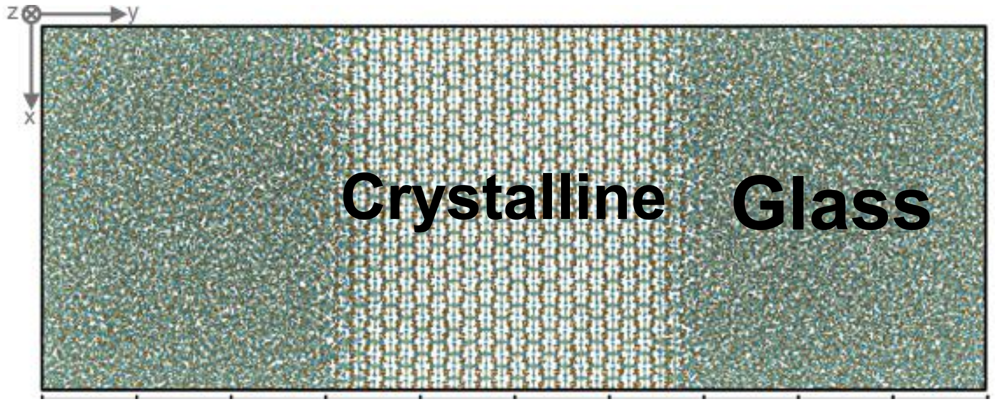
- **Mg^{2+}** cannot induce membrane condensation due to its **hydration shell** **[7]**.
- **Ca^{2+}** reduces repulsion between headgroups, inducing **membrane condensation** [7].
- As Conc. of **Ca**Cl_2 increases, portion of interfacial water (**IW**) of **Ca**Cl_2 decreases.

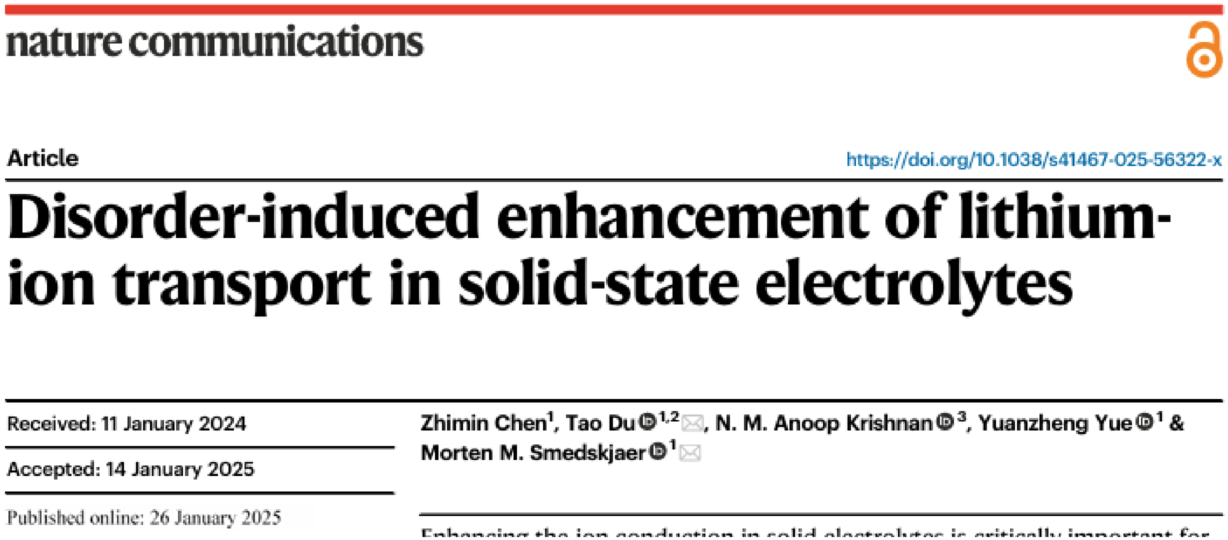
(See $\rho_{H_2O}(z)$ in **Fig. 2 (f)**)

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

SI Result 1 (c): Lateral Displacement Distribution

Li_3PS_4




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

Accepted: 14 January 2025

Published online: 26 January 2025

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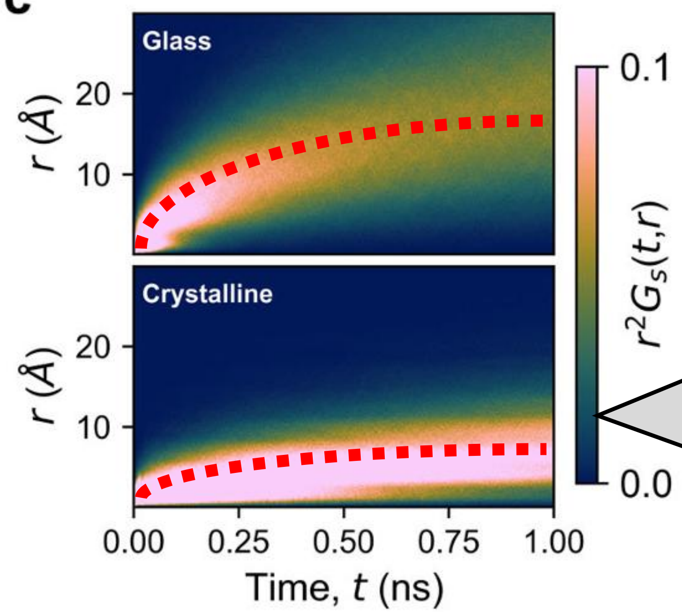
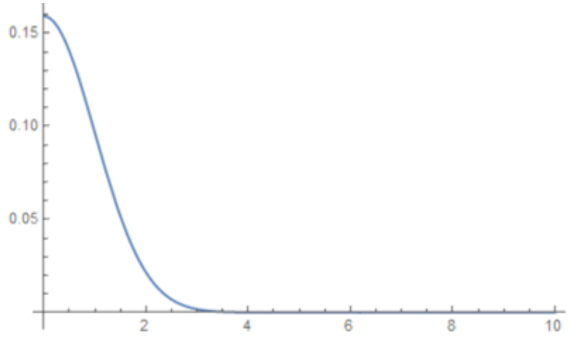
c



$2Dt\sqrt{2}$

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

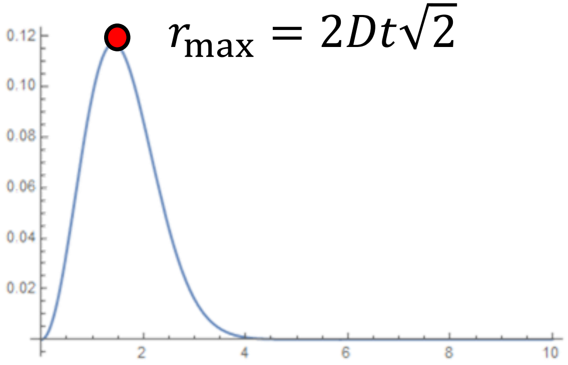
$$G_s(\boldsymbol{r},t) = (4\pi Dt)^{-3/2}e^{-r^2/4Dt}$$



r

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

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



r

SI Result 1 (c): Lateral Displacement Distribution

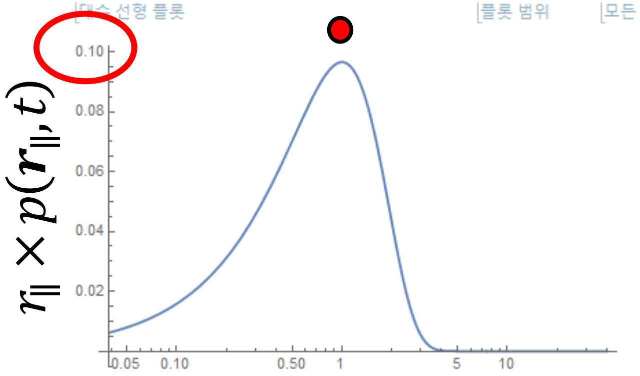
$$G_s(\boldsymbol{r}_\parallel,t) \cong \sum_n f_n G_{\mathcal{N}}\left(\boldsymbol{r}_\parallel,t|D_\parallel^{(n)}\right) \qquad \sum_n f_n = 1$$

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

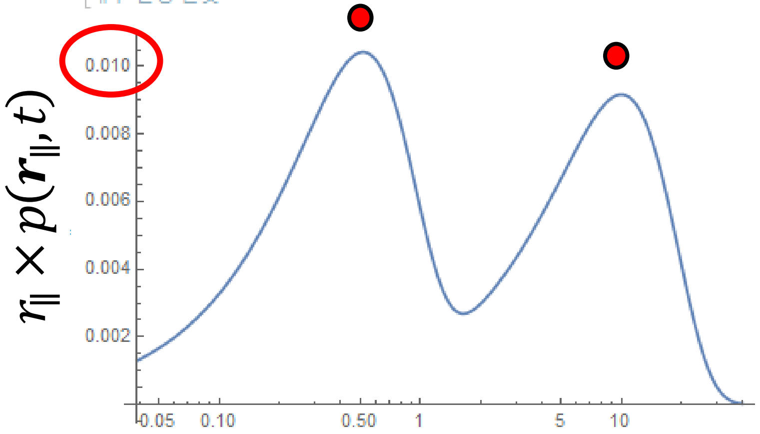
$$r_\parallel \times G_{\mathcal{N}}(\boldsymbol{r}_\parallel,t|D_\parallel) \rightarrow \text{ maximum at } r_\parallel = \sigma = \sqrt{2D_\parallel t}$$

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

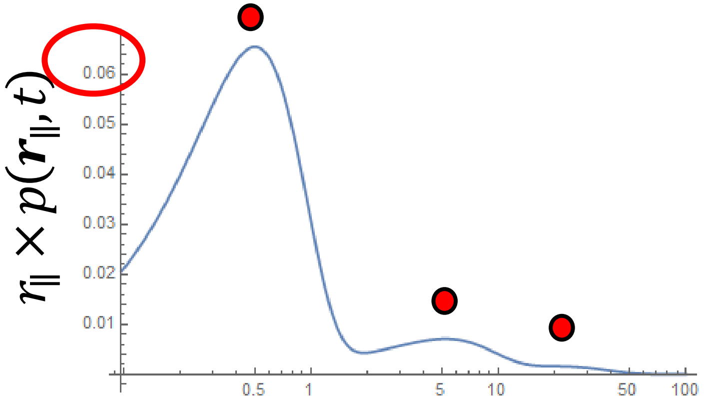
```
In[30]:= LogLinearPlot[x (P[x, 1]), {x, 0, 40}, PlotRange → All]
```
대수 선형 플롯 플롯 범위 모든




```
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

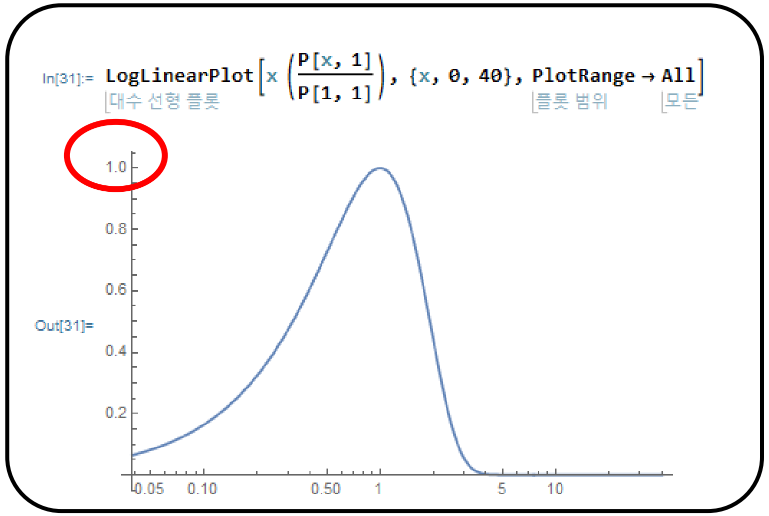


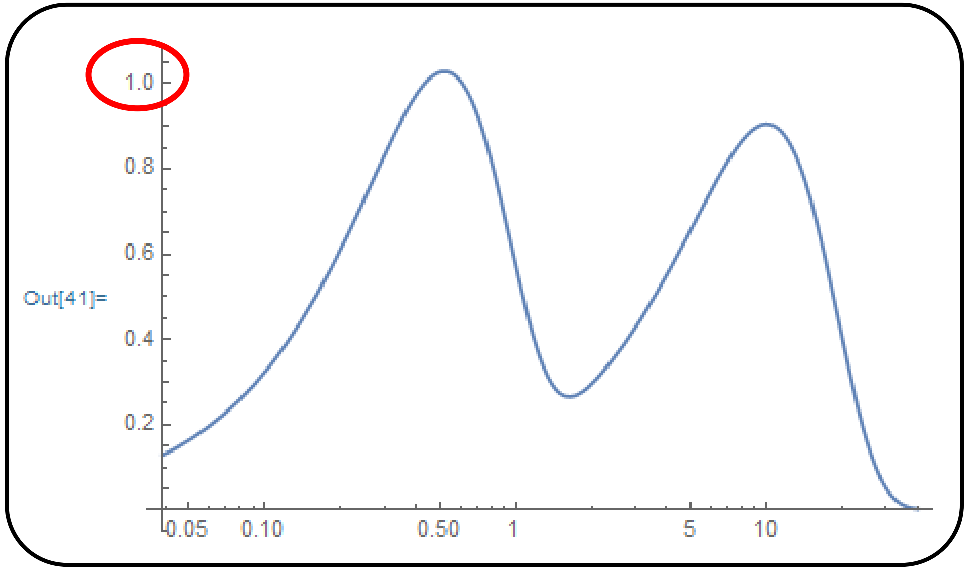
SI Result 1 (c): Lateral Displacement Distribution

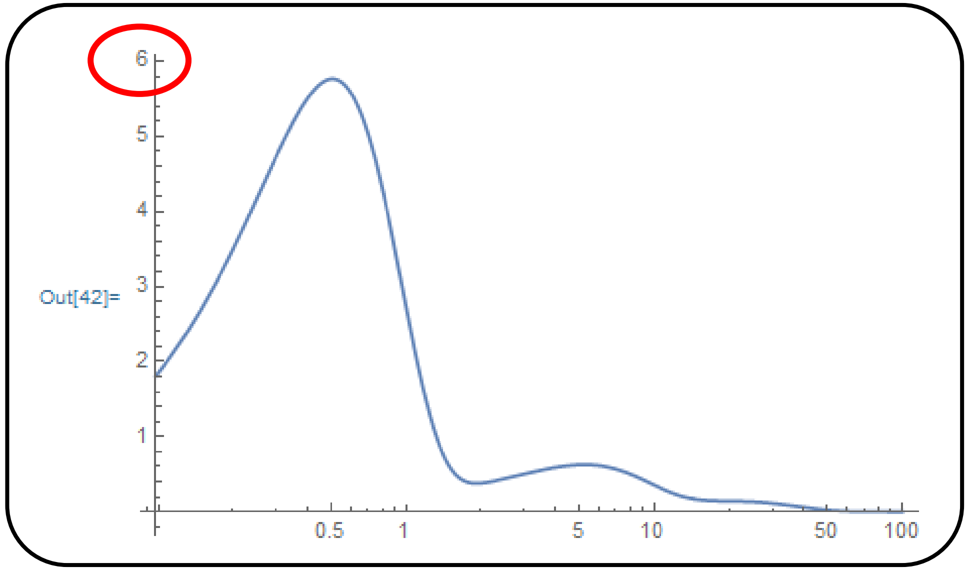
$$G_s(\boldsymbol{r}_\parallel,t) \cong \sum_n f_n G_{\mathcal{N}}\left(\boldsymbol{r}_\parallel, t \middle| D_\parallel^{(n)}\right) \qquad \sum_n f_n = 1$$

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

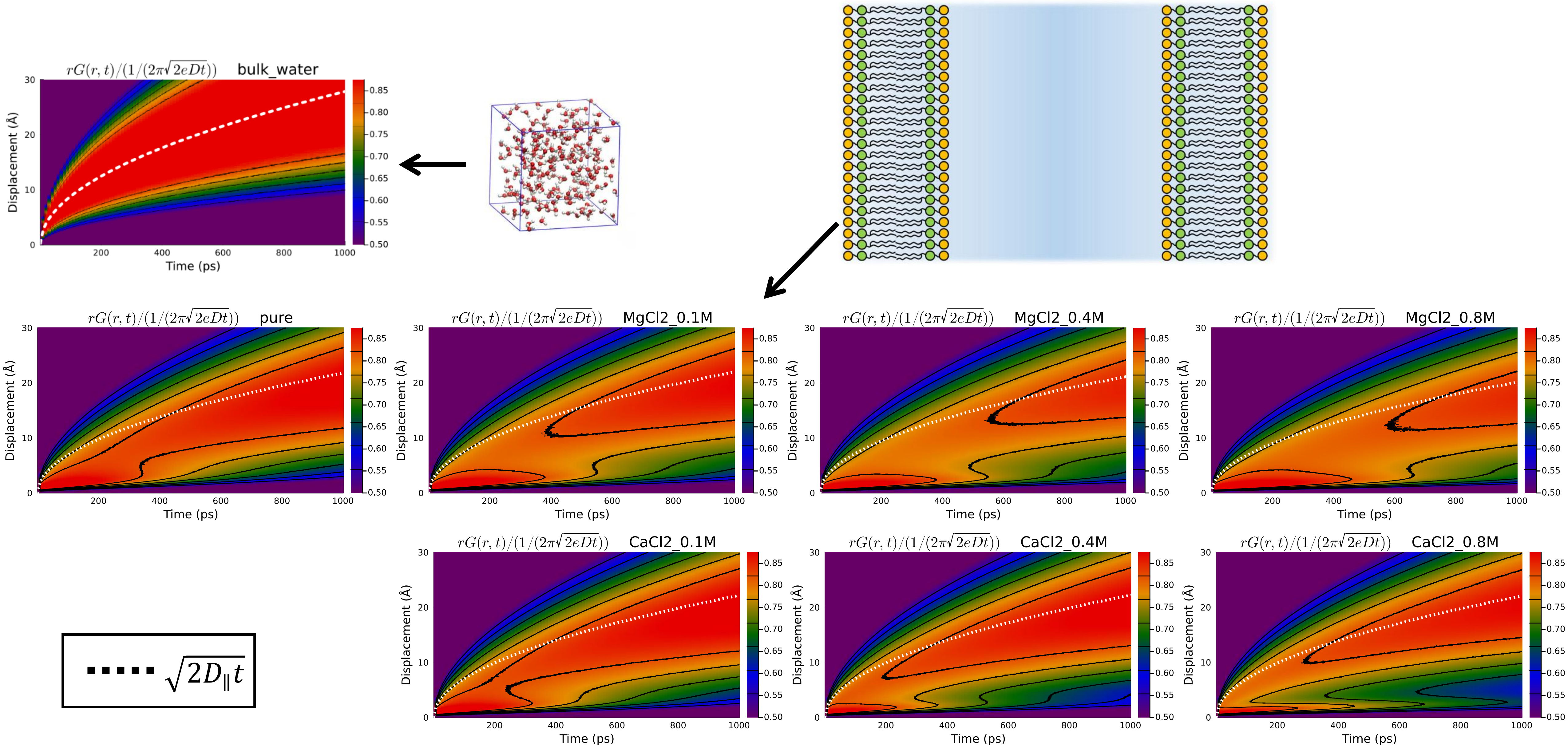
$$f(\boldsymbol{r}_\parallel,t) \equiv \frac{r_\parallel G_s(\boldsymbol{r}_\parallel,t)}{\sigma\, p_{\mathcal{N}}(\sigma,t|\sigma)}\bigg|_{\sigma=\sqrt{2\langle D_\parallel\rangle t}}$$



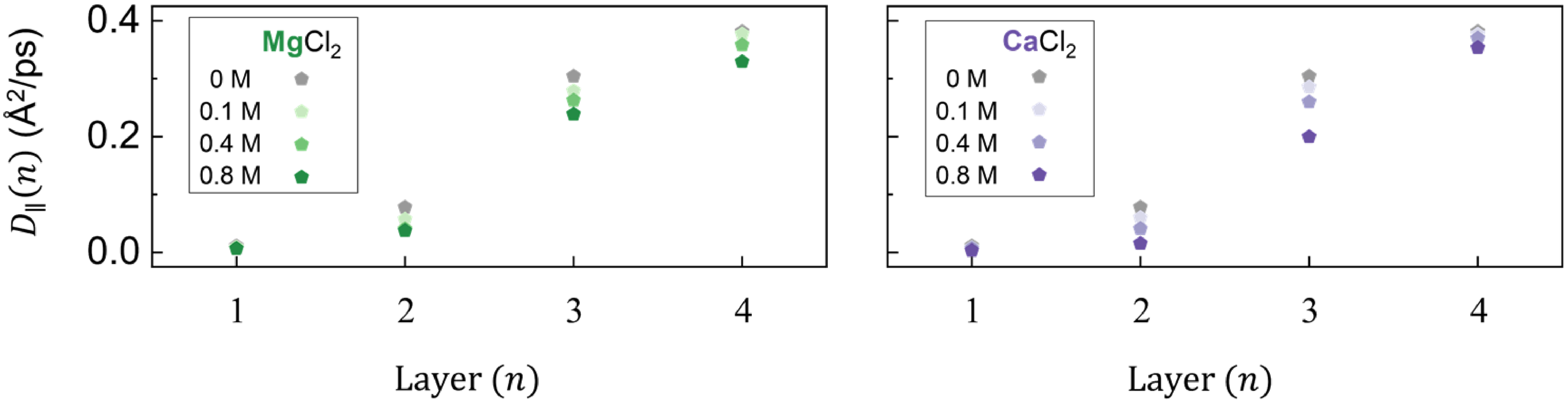




SI Result 1 (c): Lateral Displacement Distribution



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

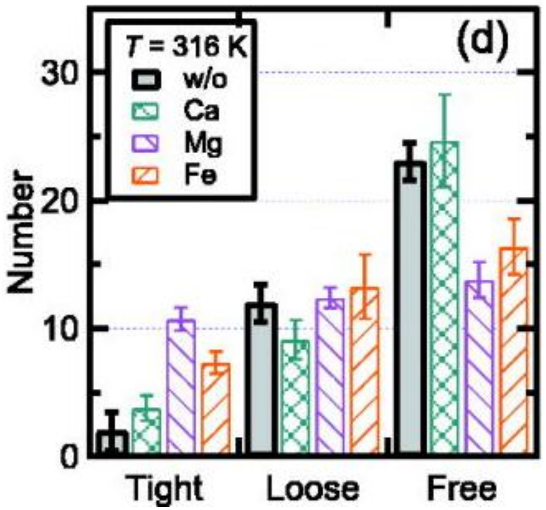


$D_{\parallel}(n)$: determined by umbrella sampling (1 μs-long)

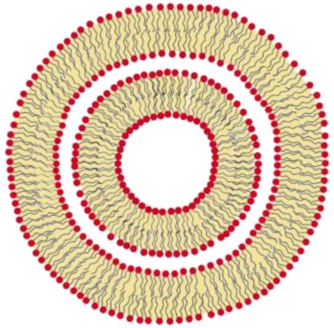
Layer(n): defined by the nodes of $\langle P_2(\cos\theta)\rangle(z)$ in the salt-free case. (see **Fig. 2 (e)**)

SI Result 1 (e): Experimental result

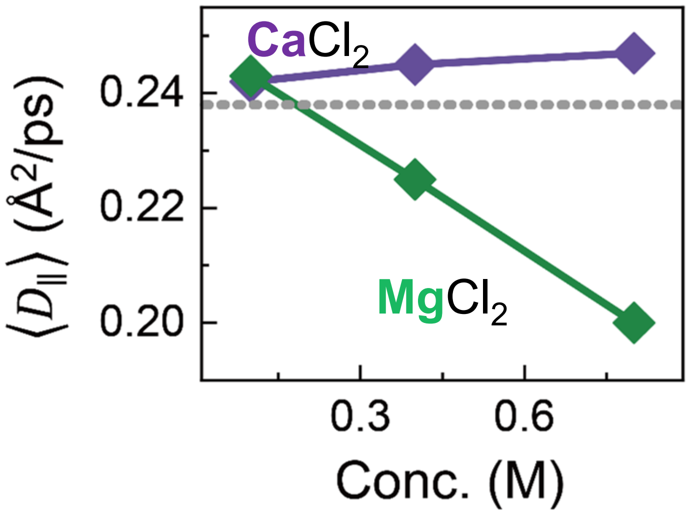
Fig. 3

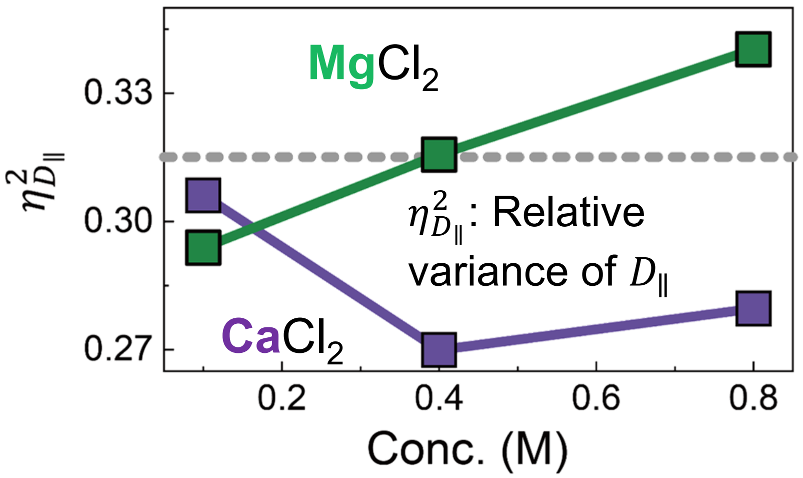


[Experiment]
DMPC
37 H_2O/lipid molecule.
0.45 M conc.



Multilamellar lipid vesicle





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

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

View Online Export Citation CrossMark

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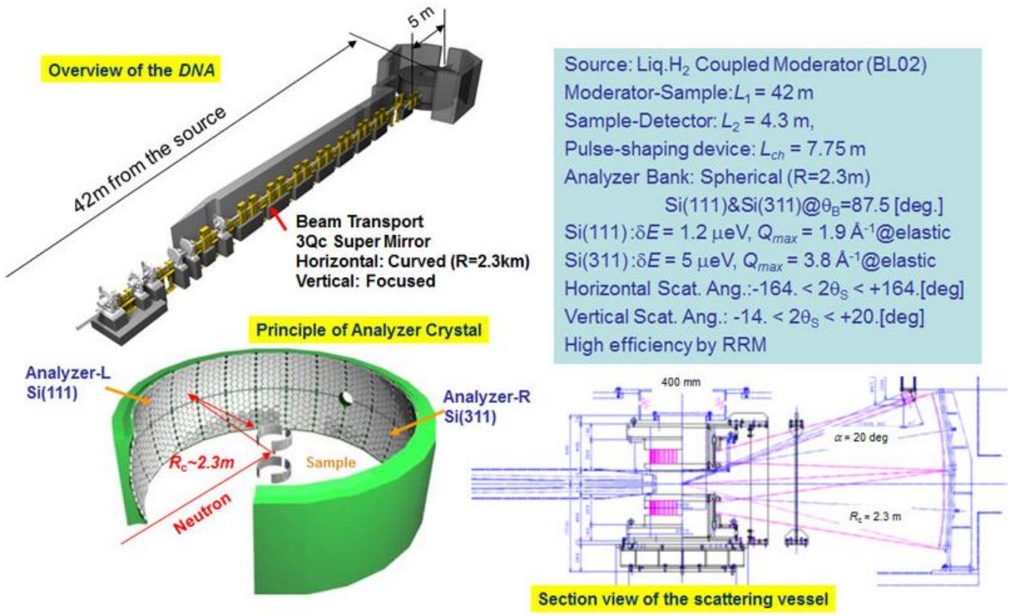

J-PARC MLF BL02 DNA: Dynamic Spectrometer