Result and Discussion

($z = 0$: the membrane center)
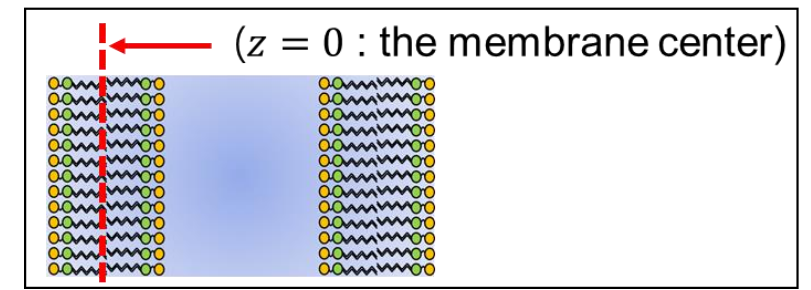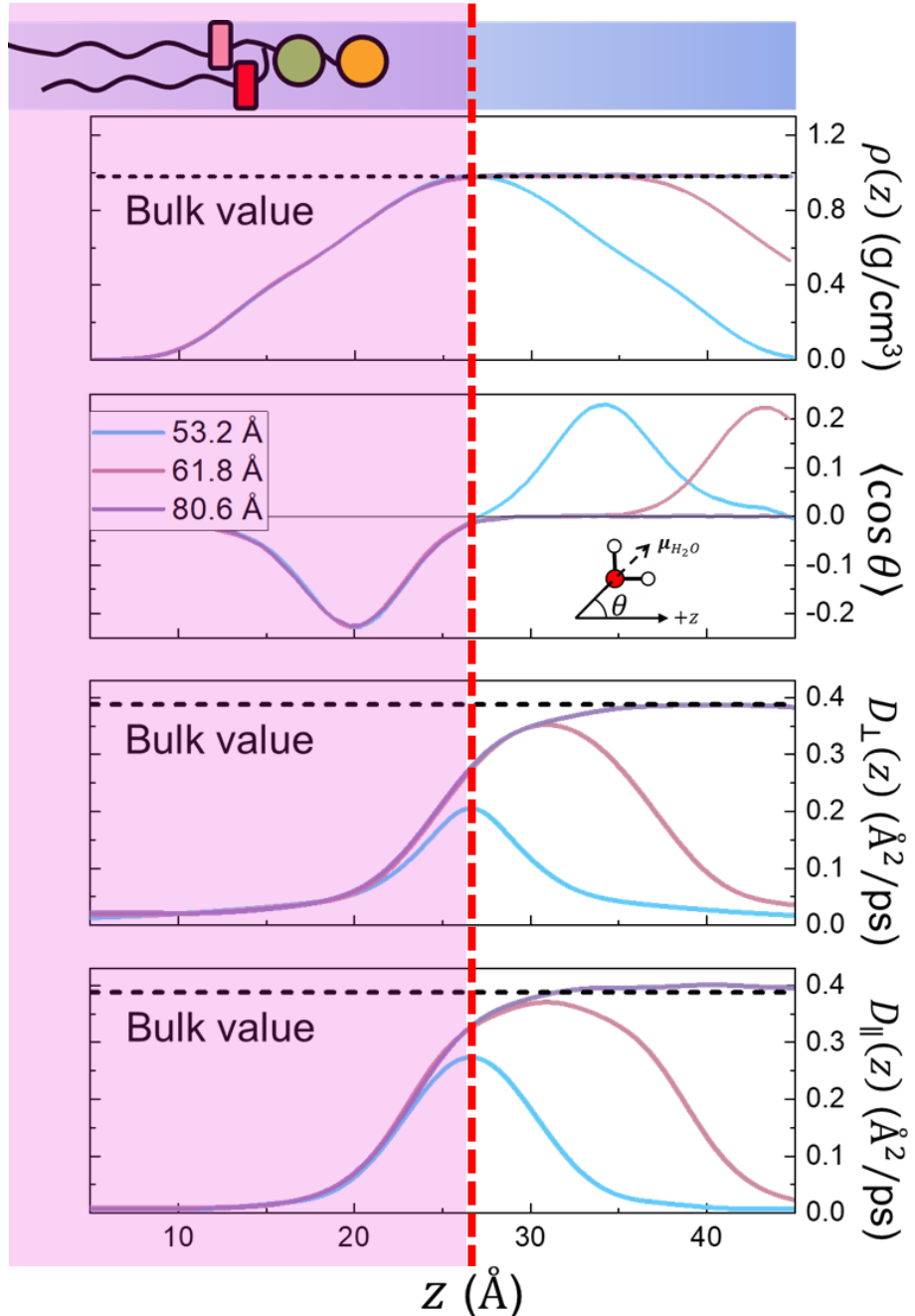
density (ρ_{H_2O})

PB Moore *et al.*, Biophysical Journal, 81, 2484-2494 (2001)

JS Hub *et al.*, Biophysical Journal, 93, 9, 3156-3168 (2007)

Water alignment information ($\langle \mu_{H_2O,z} \rangle / \langle \mu_{H_2O} \rangle$)

JA Mondal *et al., J. Am. Chem. Soc.*, 134, 18, 7842-7850 (2012)

LB Dreier *et al., J. Phys. Chem. Lett.*, 10, 20, 6355-6359 (2019)

Vertical Diffusion Coefficient ($D_\perp(z)$)

$D_\perp(z) \rightarrow$ determined from 'mean first passage time'.

Y von Hansen *et al., Phys. Rev. Lett.*, 111, 118103 (2013)

Lateral Diffusion Coefficient ($D_\parallel(z)$)

$D_\parallel(z) \rightarrow$ determined from 'result of umbrella sampling method'.

Y von Hansen *et al., Phys. Rev. Lett.*, 111, 118103 (2013)

$\ell = 53.2$ Å $\ell = 61.8$ Å $\ell = 80.6$ Å

(a) $\rho(z)$ (g/cm^3)

(b) $\beta U(z)$

(c) $\tau_{\mathrm{fp}}(z, z_t)$ (ns)

(d) $D_\perp(z)$ (Å^2/ps)

Z (Å)

(a) $\ell = 53.2$ Å $\ell = 61.8$ Å $\ell = 80.6$ Å

Row (a): $\rho(z)$ (g/cm³) vs z (Å)

Row (b): MSD (Å²) vs time (ps)

Row (c): $D_\parallel(z)$ (Å²/ps) (Before correction) vs z (Å); insets: MSD vs time, $4\langle D_\parallel \rangle t$

Row (d): $D_\parallel(z)$ (Å²/ps) (After correction) vs z (Å); insets: MSD vs time, $4\langle D_\parallel \rangle t$

DKC plot (left): $2\langle\delta\boldsymbol{v}_{x,y}{}^{2}(t)\,\delta\boldsymbol{v}_{x,y}{}^{2}(0)\rangle/\langle\boldsymbol{v}_{x,y}{}^{2}\rangle^{2}$ of bulk water

Left panel: DKC vs time (ps), with annotation $2\langle \delta \boldsymbol{v}_\parallel^2(t)\delta \boldsymbol{v}_\parallel^2(0)\rangle / \langle \boldsymbol{v}_\parallel^2\rangle^2$ of bulk water.

Right panel: NGP vs time (ps).