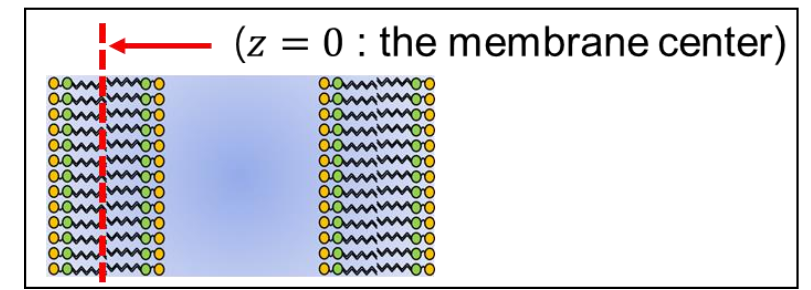
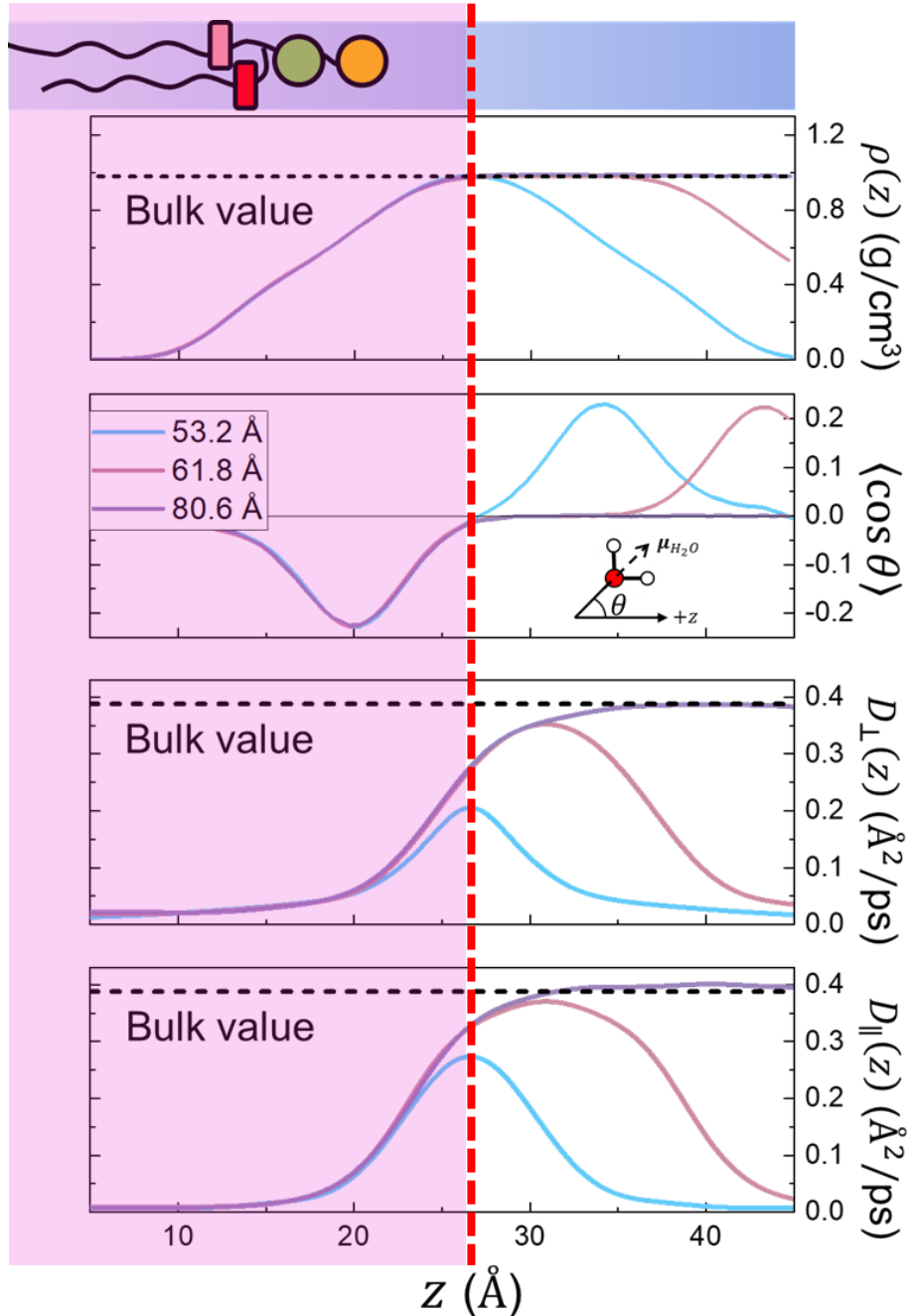


# Result and Discussion



← **density ( $\rho_{H_2O}$ )**

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)

