Supplementary Information for

Non-Continuum Intercalated Water Diffusion Explains Fast Permeation through Graphene Oxide Membranes

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This Supplementary Information Material contains

- Supplementary Figures S1-S7 and Captions

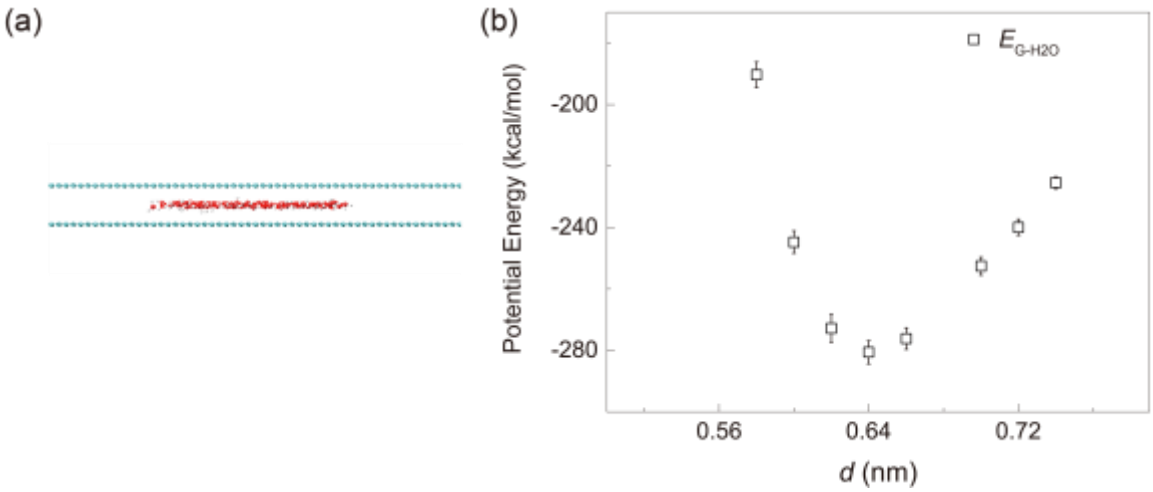

Figure S1. (a) The atomistic model with intercalated water (N_W = 115) between two flat graphene sheets with an interlayer distance d, at 300 K. (b) The potential energy of intercalated water as a function of d, with a minimum around d = 0.65 nm.

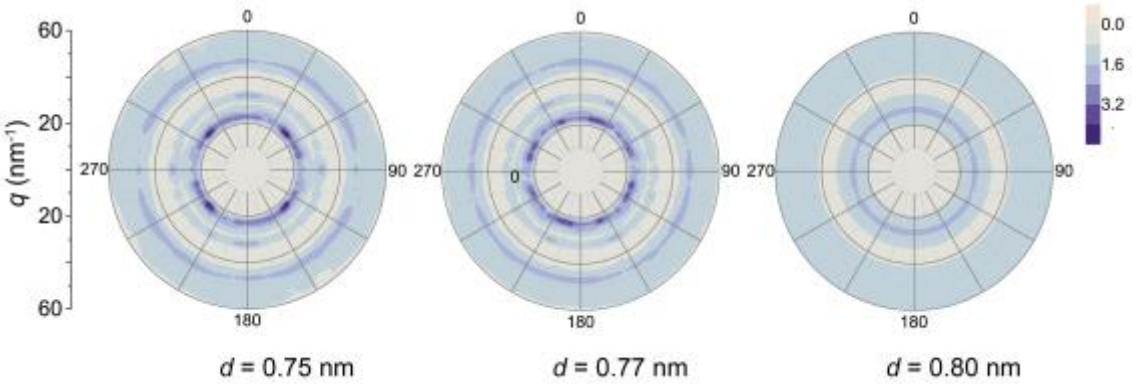

Figure S2. 2D structure factors of intercalated water between graphene layers, calculated at T = 300 K, d = 0.75, 0.77, 0.8 nm and N_W = 221.

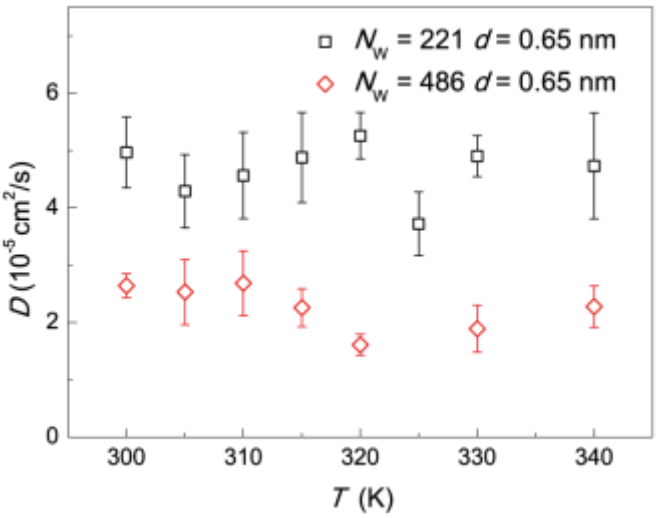

Figure S3. The dependence of collective diffusion coefficients D for the intercalated water on T with N_W = 221, 486 and d = 0.65 nm.

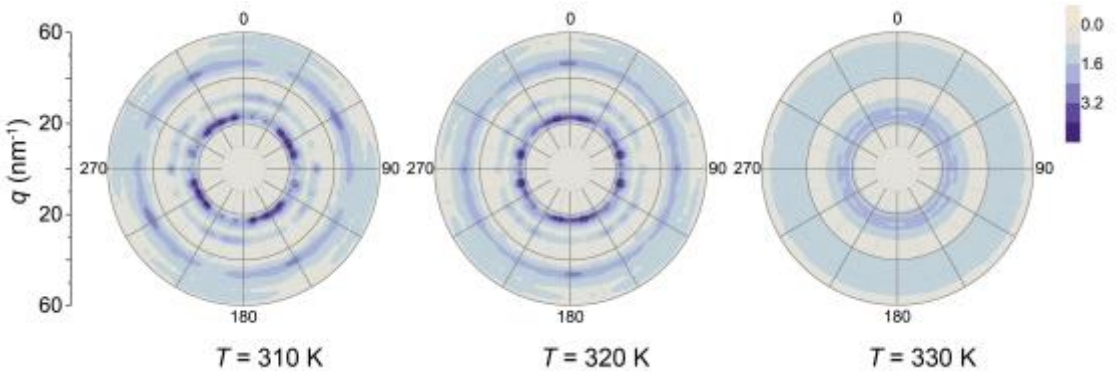

Figure S4. 2D structure factors of intercalated water between graphene layers, calculated at T = 310, 320, 330 K at d = 0.65 nm and N_W = 221.

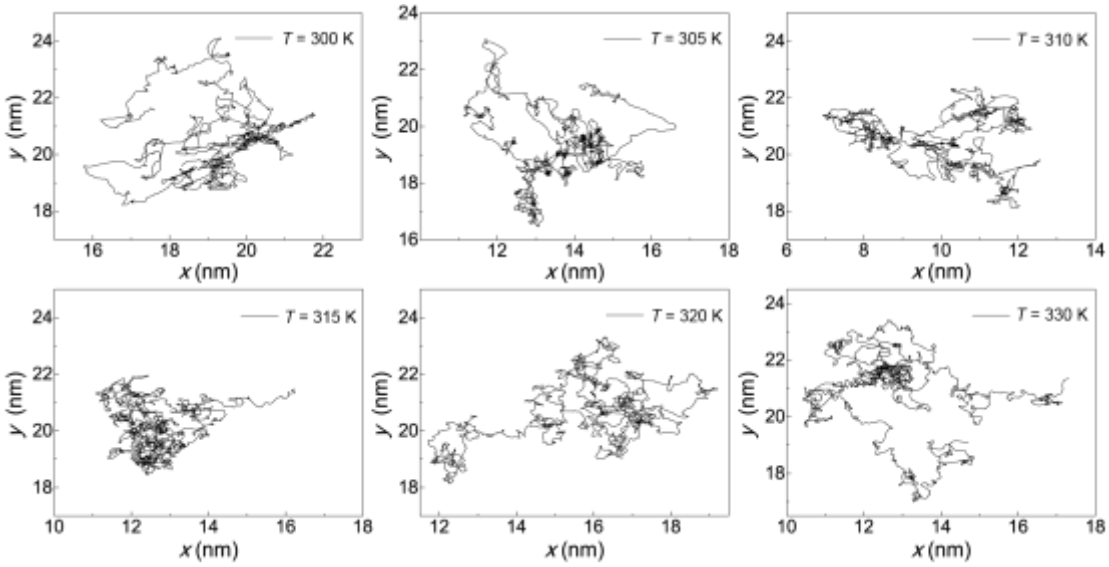

Figure S5. Center-of-mass trajectories of intercalated water in a 10 ns simulation, plotted with a time step of t_d = 10 ps. The results show deviation from the Gaussian behavior at T below the solid-fluid transition temperature T_c = 315 K. Above T_c, the Gaussian-like diffusion behavior is recovered.

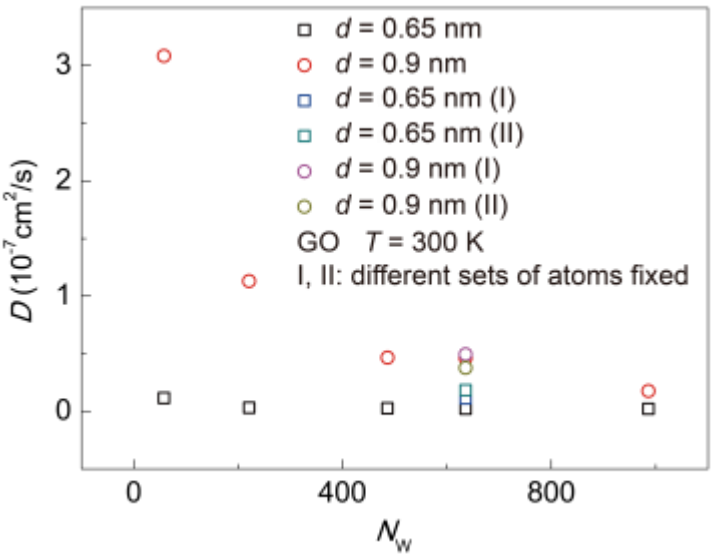

Figure S6. The dependence of D on N_W and compare results of the structure with partial carbon atoms (three of them are chosen from the sample randomly) fixed at d = 0.65 nm, d = 0.9 nm and T = 300 K.

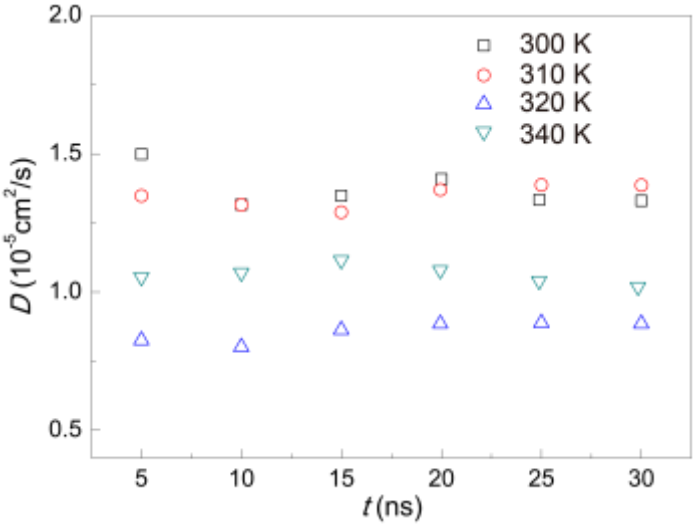

Figure S7. The convergence of collective diffusion coefficients *D* over simulation time at different temperature with N_W = 986, *d* = 0.65 nm.