Supporting Information

Molecular Insight into Water Transport through Heterogeneous GO-based Two-Dimensional Nanocapillary

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Models and initial configuration

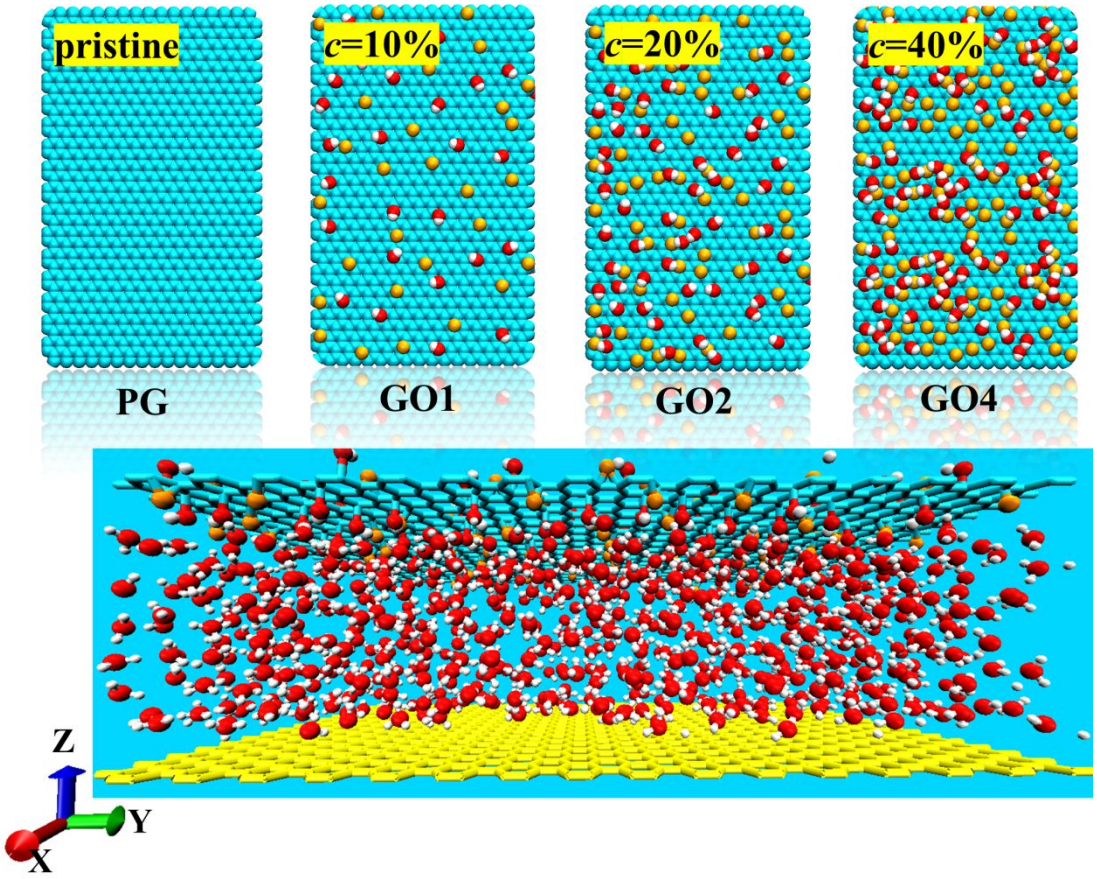

Figure S1. (Top panel) Front view of the four GO sheets used in our MD simulations (pristine graphene, grphene oxide with oxidization concentrations being 10%, 20% and 40%, respectively). (Bottom panel) Lateral view of the simulation system of GO pore model in which the channel is constructed by combining various GO sheets. Color code: C in the GO sheet: cyan and yellow; O in epoxy: orange; O in the hydroxyl and water: red; H in hydroxyl of water: white.

Flow rate vs. applied pressure

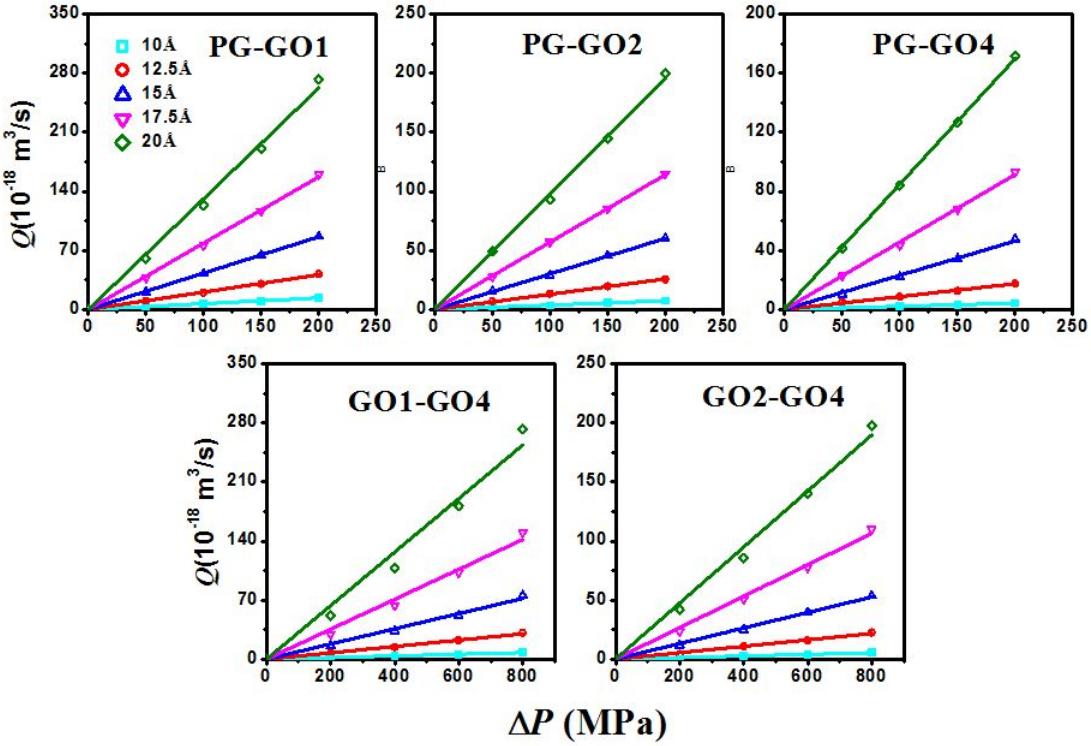

Figure S2. Volumetric flux as a function of applied pressure for the five heterogeneous pore models, where the scatters represents for the MD simulation results and the solid line denotes for the linear fitting plot of relation between flux and driven pressure. The volumetric flow rate (*Q*) was calculated from the average streaming velocity in the confined pore ($Q=\bar{v}Wd_{eff}$). In the calculation equation, $\bar{v}$ is the average streaming velocity obtained from the flowing velocity profiles under stable flow state, *W* is the width of the channel and d_{eff} is the effective pore size, which excludes the half thickness of the both wall sheets.

Sensitivity analysis of slip length

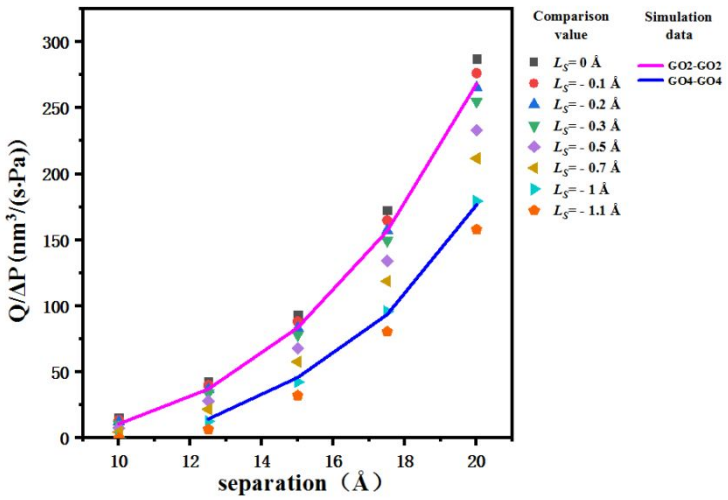

Figure S3. Variation of Q/Δ*P* with the slip lengths for two homogeneous GO channels under different separations.

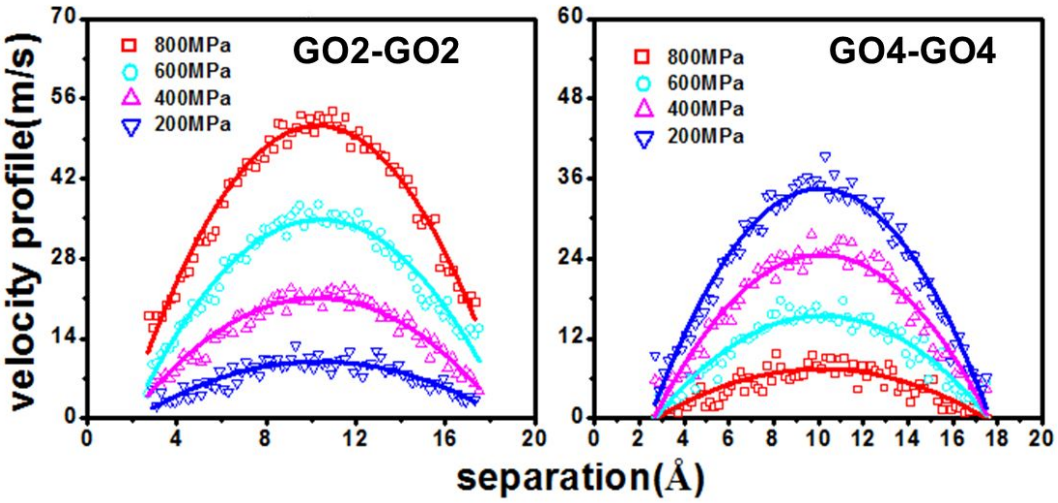

Figure S4. The velocity profiles of water molecules in different homogeneous GO channels with interlayer distance of 20Å under various pressures; the solid line is the correlated velocity distributions via the derived velocity expression (Equation 3). In the computation of simulated velocity distribution, just like the density profile, the crossing area of GO channels was divided many small bins, in which the average water velocity was statistically calculated based on the simulated velocity of each water molecule located within each bin.

Theoretical and simulated velocity profiles

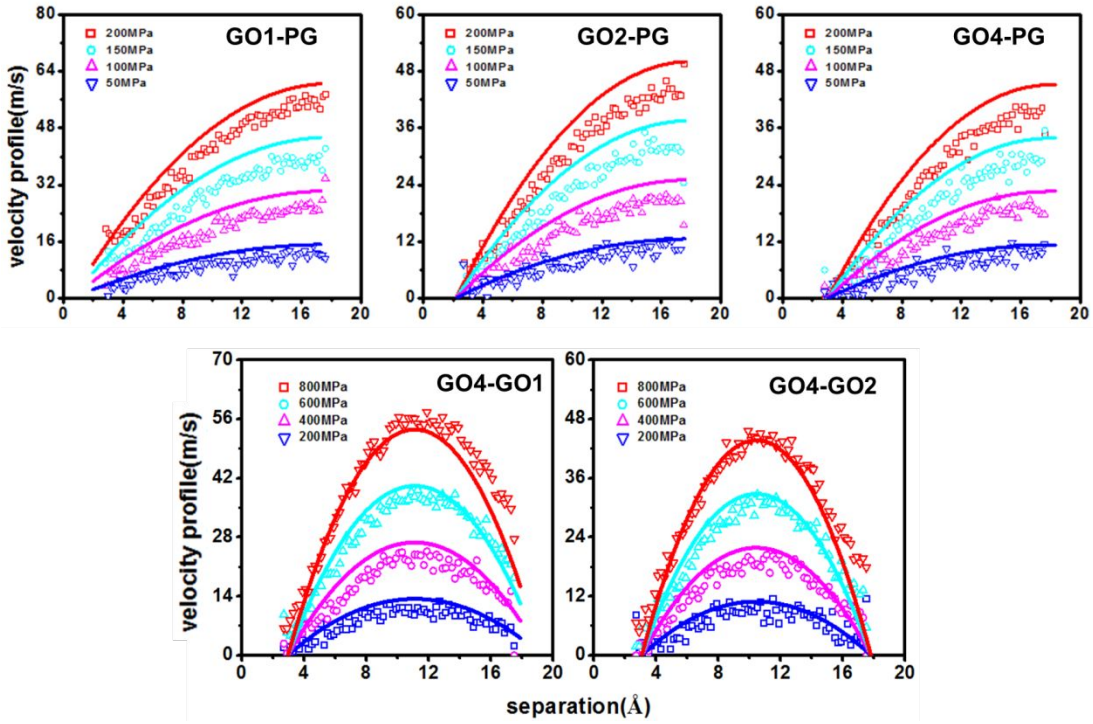

Figure S5. The velocity profiles of water molecules in different heterogeneous GO channels with interlayer distance of 20Å under various pressures; the solid line is the predicted velocity distributions via the derived velocity expression (Equation 3).

Interfacial water configuration

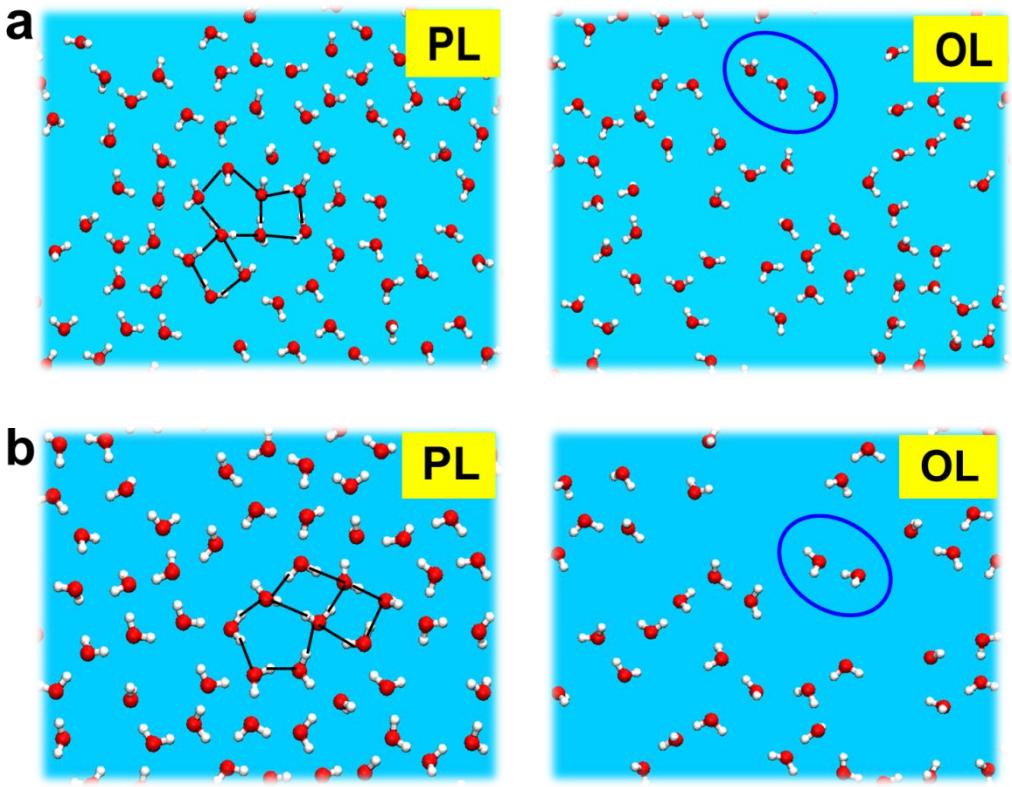

Figure S6. Atomic snapshot structures of water molecules inside the two interfacial hydrolayers (PL and OL) for PG-GO2 pore with the interlayer distances of 10Å (a) and 20Å (b).

Potential energy surface (PES)

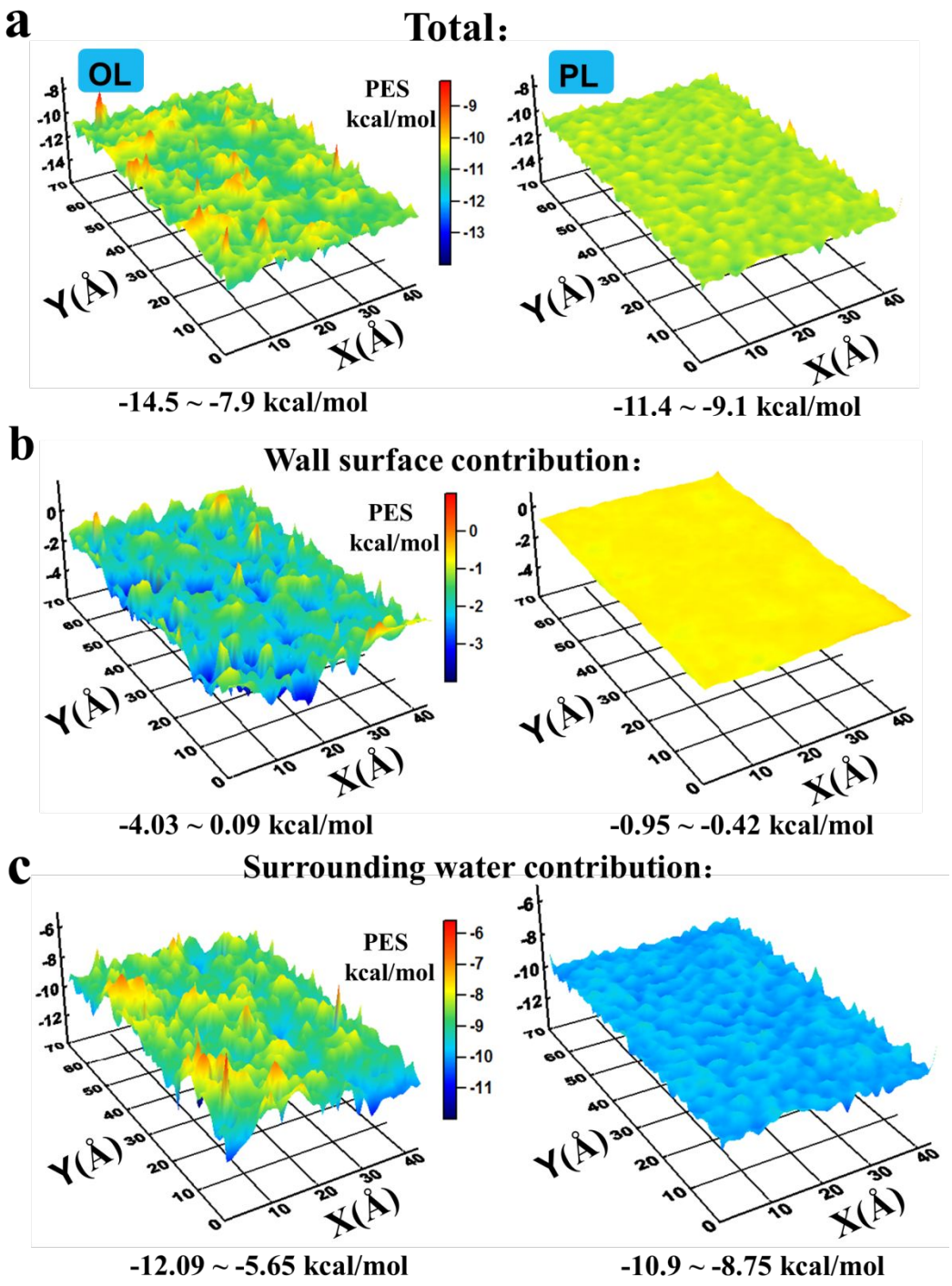

Figure S7. (a) the potential energy surface (PES) per water molecule in PL and OL for the 10Å PG-GO2 pore, and its decomposition into the solution-induced contribution (b) and the wall sheet interaction contribution (c).

Hydrogen bond density

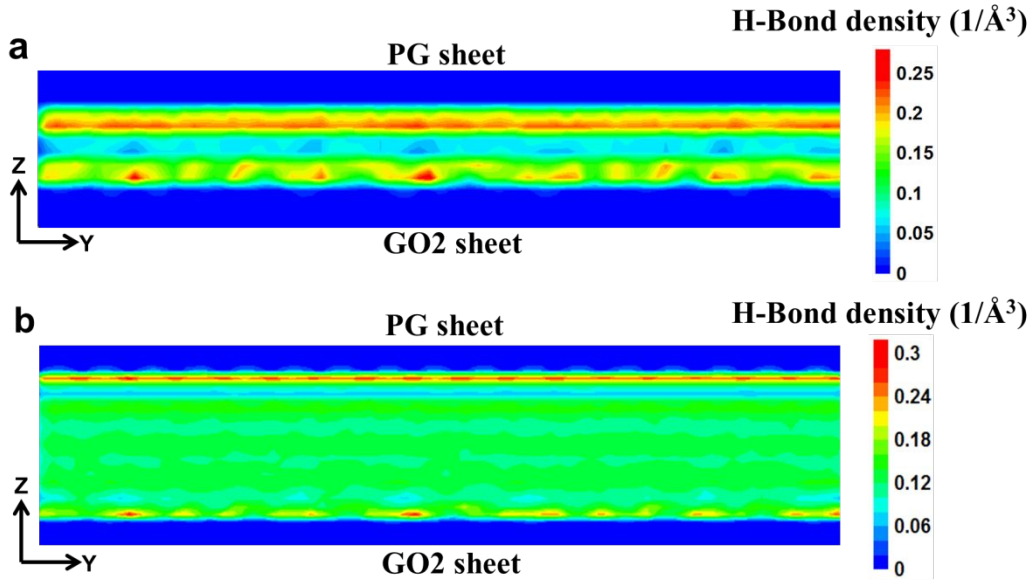

Figure S8. The HB density distributions of water in the Y-Z plane for the PG-GO2 pore with the interlayer distance of 10Å (a) and 20Å (b). According to the HB density profile, it is observed that water molecules near PG sheet exhibit a higher and well-ordered HB distributions compared to interfacial hydrolayer near GO2 sheet, which might result from the destruction of water-water HB network in OL. This result corresponds to the 2-D HB landscapes (Figure 7) and the 2-D water density profiles (Figure 6).