Supplementary Material

Specific Heat Capacity of Confined Water in Extremely Narrow Graphene Nanochannels

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Content

1. Independence checks

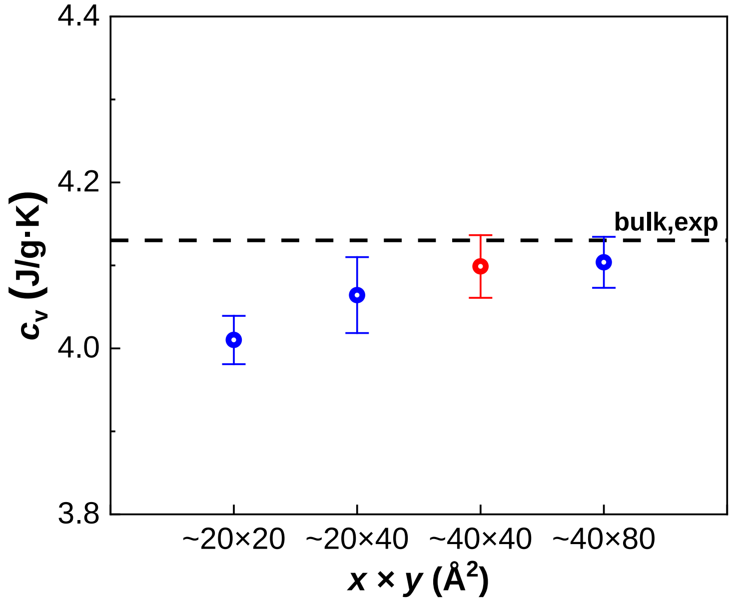

Figure S1 Independence check for box size. A box size of about 40 × 40 Å is precise enough to eliminate the boundary effects.

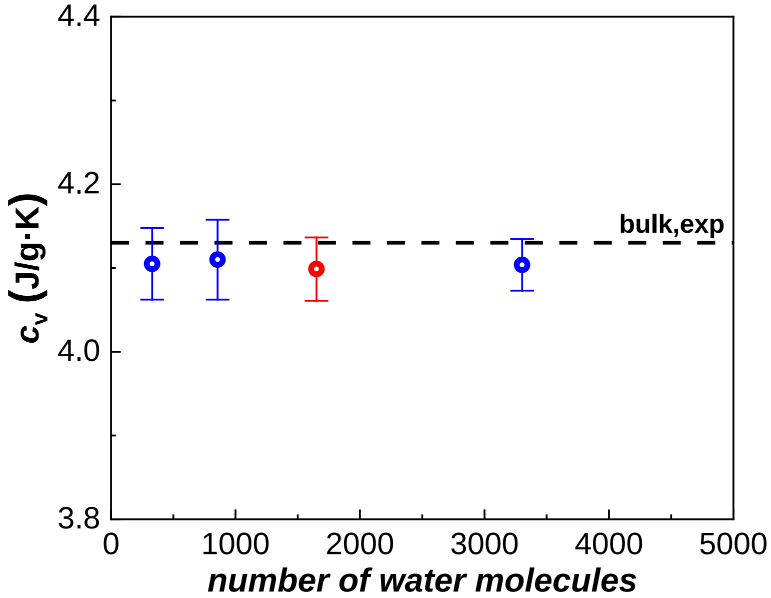

Figure S2 Independence check for number of water molecules. The specific heat capacity is not sensitive to the number of water molecules.

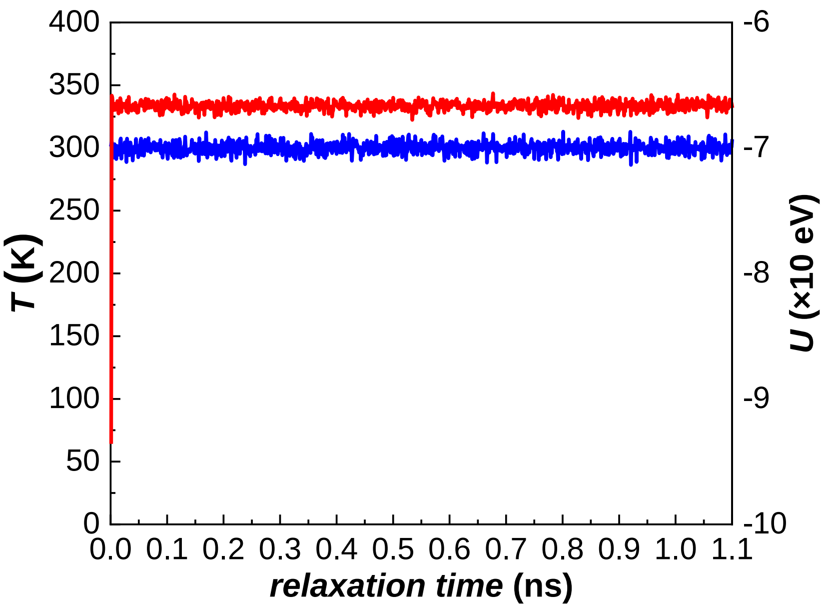

Figure S3 Independence check for relaxation time. Both temperature and internal energy of the simulation system converge fast. Thus, a relaxation time of 1.1 ns is long enough to reach an equilibrium state.

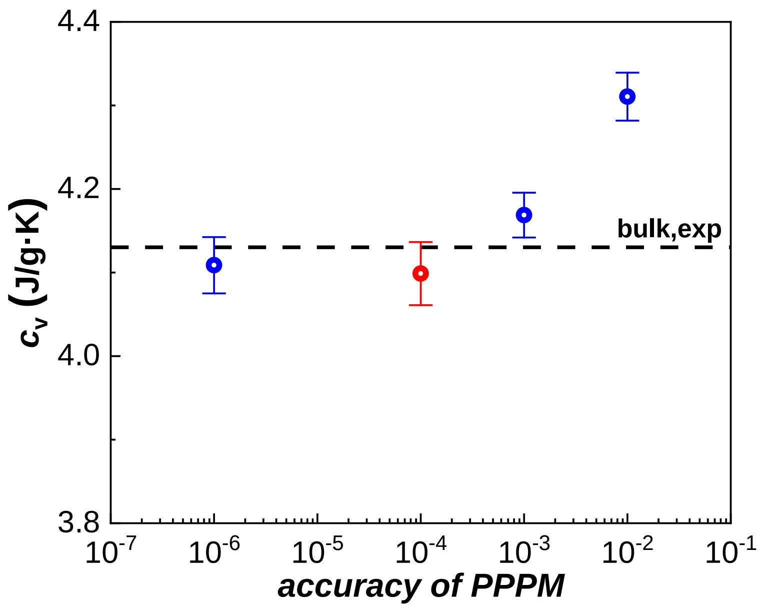

Figure S4 Independence check for accuracy of PPPM. A convergence accuracy of 10^{-4} of PPPM is precise enough to match the experimental value of specific heat capacity of bulk water and thus is chosen in this work.

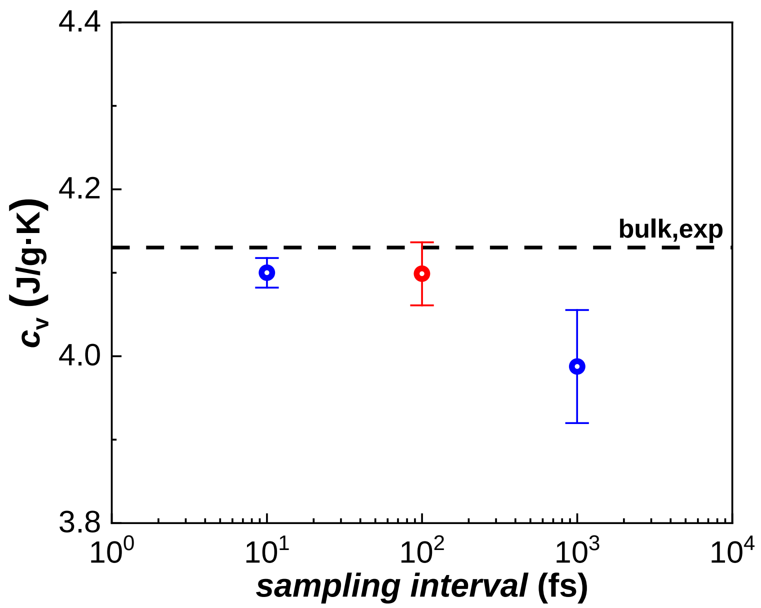

Figure S5 Independence check for sampling time. A sampling interval of 100 fs is precise enough to match the experimental value of specific heat capacity of bulk water and thus is chosen in this work.

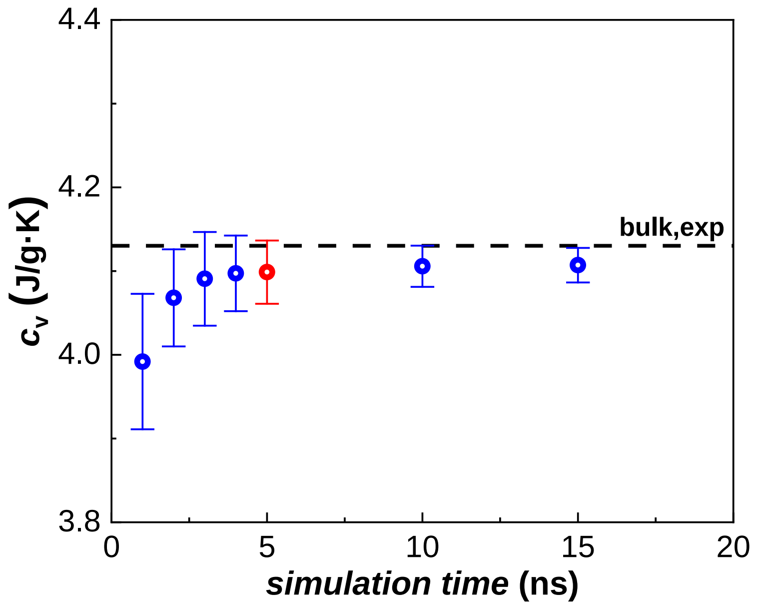

Figure S6 Independence check for simulation time. A simulation time of 5 ns is long enough to match the experimental value of specific heat capacity of bulk water and thus is chosen in this work.

2. Density Distribution

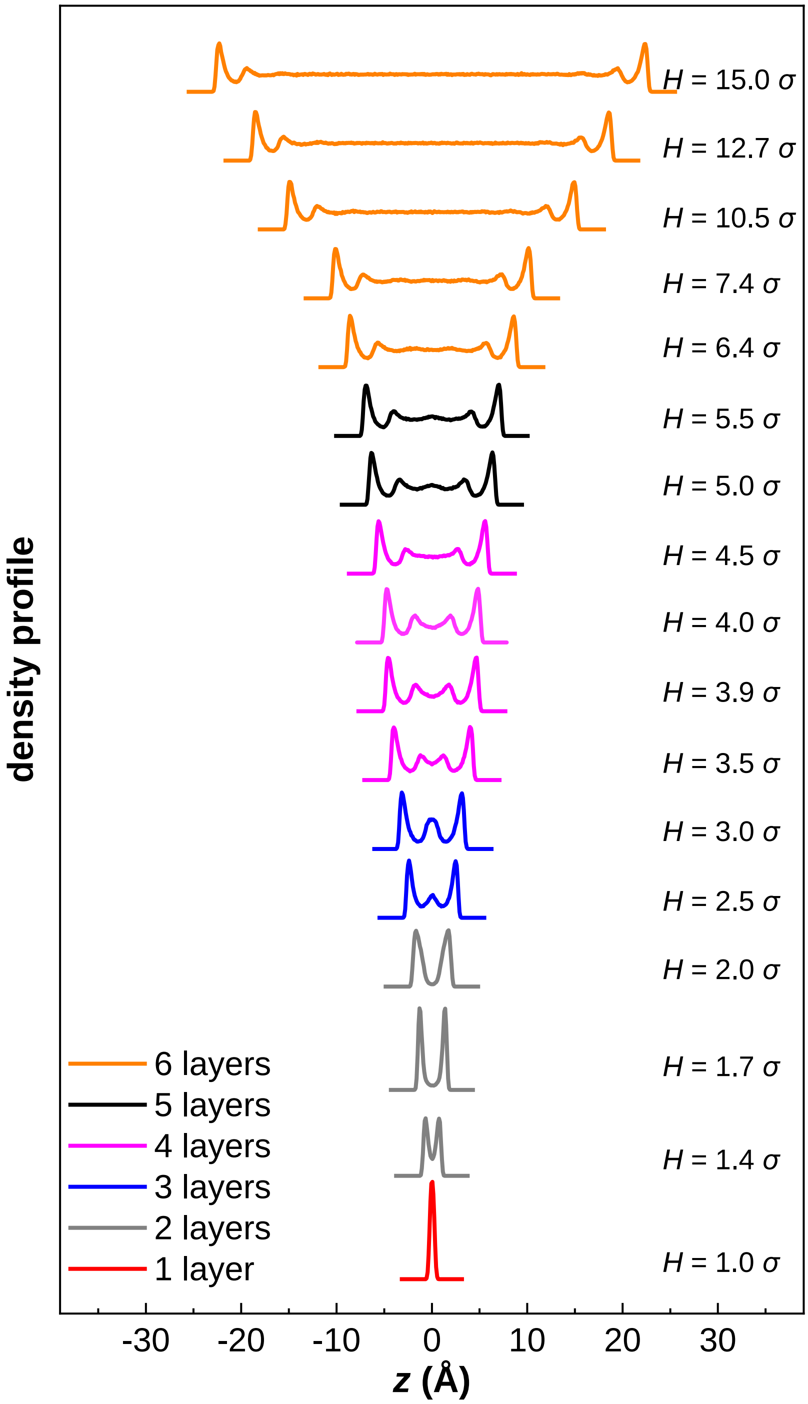

Figure S7 Density distributions of water in nanochannels. Water forms as layers in nanochannels where a density peak corresponds to a water layer. The number of water layer can be the same at different channel heights within a certain range but the distance among them are difference. Thus, the properties of water including c_v oscillate on local.

3. Radial Distribution Function $g(r)$

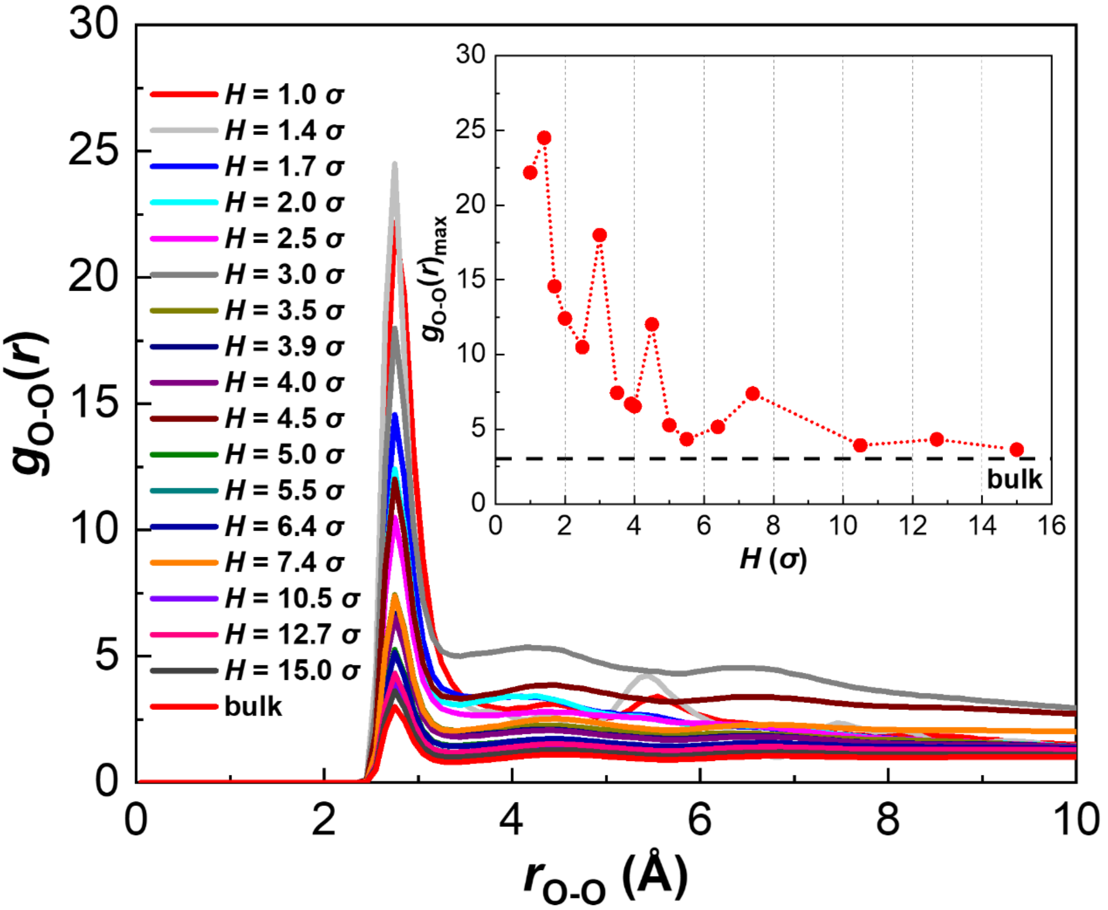

Figure S8 Radial distribution function $g_{O\text{-}O}(r)$ of water molecules (take oxygen as example) in nanochannels. The negative relationship between c_v of water confined in different nanochannels and the first peak of $g_{O\text{-}O}(r)$, namely, $g_{O\text{-}O}(r)_{max}$ in the inset, explain the size-dependent c_v of nanoconfined water. And the local highest $g_{O\text{-}O}(r)_{max}$ generally corresponding to the local lowest c_v explains the commensurability of c_v.

4. High n_{hbond} in the nanochannel of H = 1.4 σ

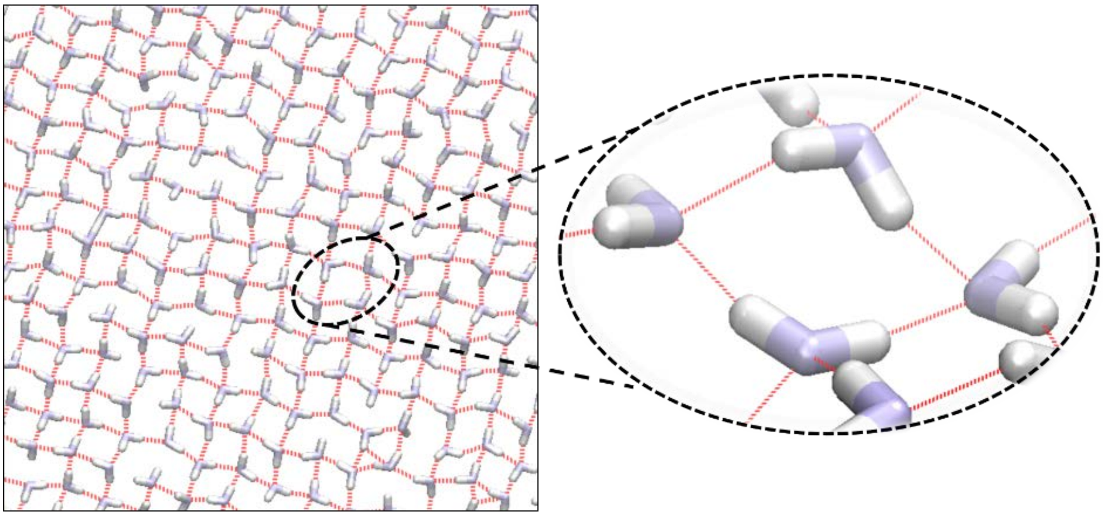

Figure S9 Special structure of confined water in channel of H = 1.4 σ. Generally, n_{hbond} in nanoconfined water are lower than the bulk value. However, in the channel with height of 1.4 σ, n_{hbond} is abnormal and extraordinarily high, reported as 3.45016 ± 0.04807, causing by its special structure, which allows water molecules connecting with hydrogen bonds sufficiently.