Supporting Information

How pressure affects confined water inside different nanoslits

Qingyin Zhang[1,*], Xin Wang[1], Jipeng Li[2], Sumin Lu[1], Diannan Lu[2,*]

[1] State Key Laboratory of Separation Membranes and Membranes Processes, School of Chemistry and Chemical Engineering, Tianjin Polytechnic University, Tianjin, 300387

[2] State Key Laboratory of Chemical Engineering, Department of Chemical Engineering, Tsinghua University, Beijing, 100084

To whom it corresponds: zhangqingyin@tjpu.edu.cn; ludiannan@tsinghua.edu.cn;

MODELS AND METHODS

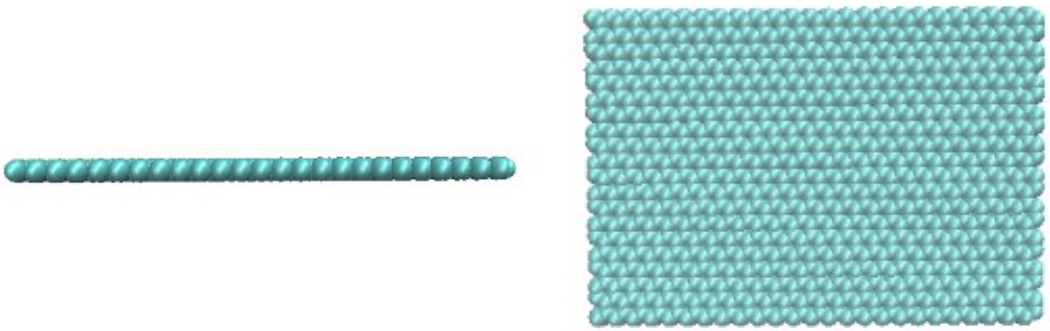
Models

All nanoslits consists of two rectangle plates with spacing distance of 0.7 nm. All models are generated using VMD package. The nanoslit was located in the center of simulation box. Water molecules were filled into the simulation box using VMD package with the density of about 1.0 g/mL. Water molecules can freely enter into or leave from nanoslits through the cross section of *x*-*y*.

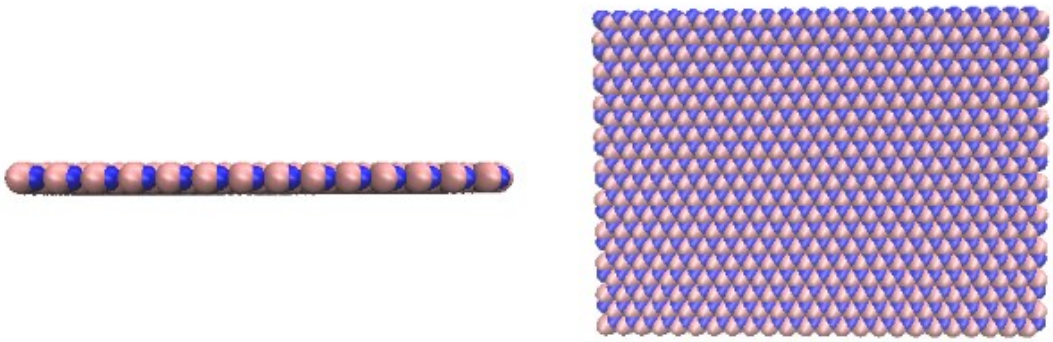
Detailed information of simulation box sizes is given in Table S1. Nanoslits were at the center of simulation boxes and water molecules are randomly added into the simulation box with bulky density of 1.0 g/mL at 1 bar. Water molecules can enter into and leave off nanoslits freely. The morphologies of graphene, hBN and MoS_2 are given in Figure S1.

Table S1 The number of water molecules and simulation box sizes of different nanoslits (Box size and the number of water inside nanoslit change with different pressure, information provided is the case of 300K and 1bar)

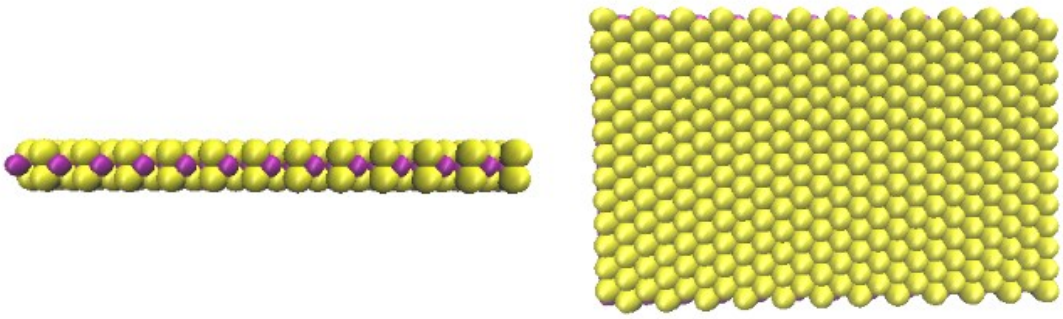
Nanoslit	Box size *x* nm × *y* nm × *z* nm	Number of water molecules inside nanoslits	Number of water molecules inside simulation box
Graphene	4.2 × 7.3 × 11.4	293	10064
hBN	4.2 × 7.3 × 11.3	294	10064
MoS_2	4.7 × 7.1 × 10.9	296	10064



(a) Graphene (left: side view; right: top view)



(b) hBN (left: side view; right: top view)



(c) MoS_2 (left: side view; right: top view)

Figure S1: Representative simulation snapshots for the monolayer structure of different nanoslit surfaces (graphene, hBN and MoS_2). Color code for atoms: Carbon - cyan; Boron - pink; Nitride - blue; Molybdenum - purple; and Sulfur - yellow.

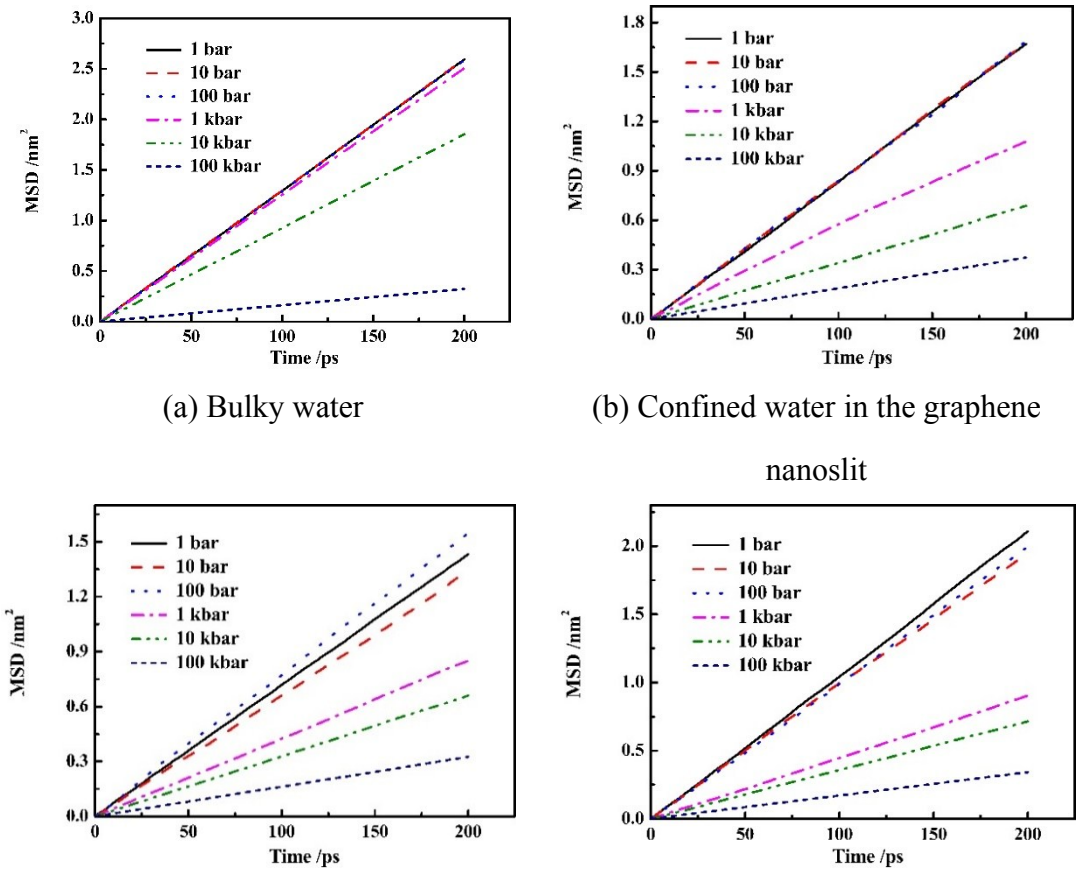
In order to help readers to reproduce our simulation work. The source files are given as appendixes, including conf file, pdb file, and psf file.

RESULTS AND DISCUSSION

Transport properties of confined water molecules in different nanoslits

The effect of pressure on the self-diffusion coefficient

The self-diffusion coefficient is calculated according to the slope of MSD with time, as shown in Figure S2.



(a) Bulky water

(b) Confined water in the graphene nanoslit

(c) Confined water in the hBN nanoslit

(d) Confined water in the MoS_2 nanoslit

Figure S2 MSD of confined and bulky water at different pressures.

It is shown that in all cases, the MSD linearly increases with time. The values of R^2 are ranged from 0.99993 to 0.9999. The diffusion coefficients in Figure 6 were calculated according to the slope of MSD with time.