Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Table S1. Sizes of simulation boxes.

interlayer spacing (Å)	**9**	**10**	**11**	**12**
box size (nm^3)	3.5 × 4.75 × 17	3.5 × 5.15 × 17	3.5 × 5.55 × 17	3.5 × 5.95 × 17

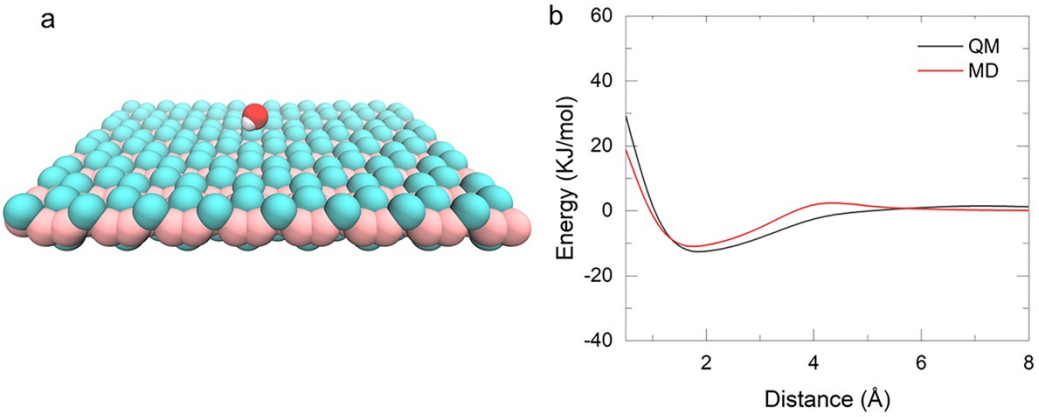

Figure S1. (a) The structure of boridene sheet and a water molecule used to fit the force fields of boridene. (b) The binding energy between the water molecule and boridene fitting in quantum modeling (QM) and in molecular dynamics (MD) simulation. The distance denotes the vertical distance between boridene surface and water molecule. The water molecule was vertically pulled upward in QM, during which a binding energy curve was obtained (black). Then, by fixing the atomic charges of Mo and B in boridene (achieved from DDEC6), we change the LJ parameters of boridene and also pull the water molecule up in MD simulation, and we achieve an appropriate set of LJ parameters, with which the binding energy curve in MD closely matches that from QM.

Table S2. Force fields of boridene.

	σ (nm)	**ε (kJ/mol)**	**charge**
molybdenum	0.415	0.7	0.405
boron	0.24	0.5	-0.27

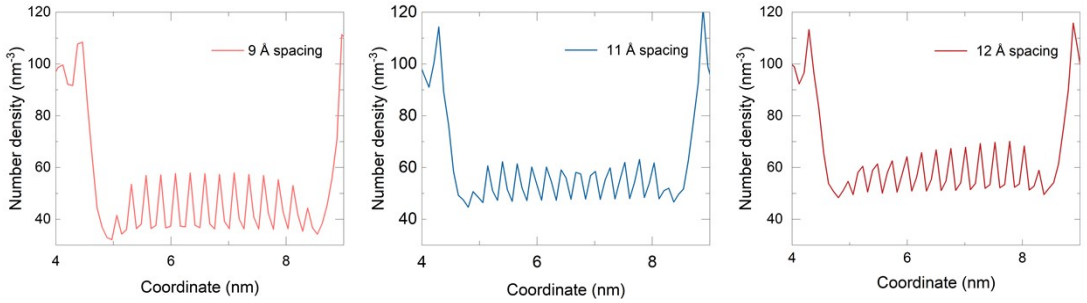

Figure S2. Local distribution of water density along the water flow direction confined inside boridene nanochannels with interlayer spacings of 9, 11 and 12 Å.

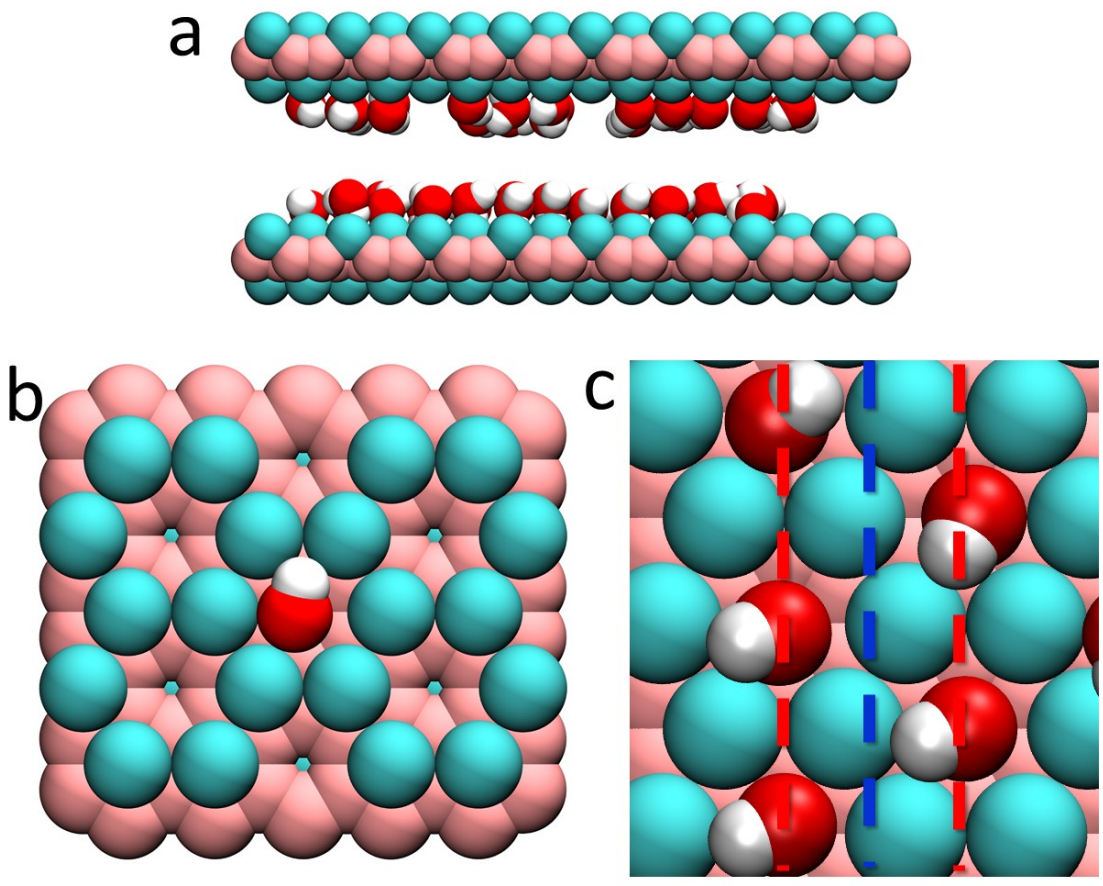

Figure S3. (a) The ordered and preferential adsorption of water at the surface of boridene. (b) Local conformation of a water molecule binding on the boridene surface with hydrogen orienting towards the groove of boridene surface. (c) Ordered water molecules trapped on the boridene surface. The red and blue dashed lines indicate the peaks and valleys in density distribution profile. The snapshots are obtained from the conformation at the final frame of the simulation under 12 Å interlayer spacing

and 100 MPa pressure.

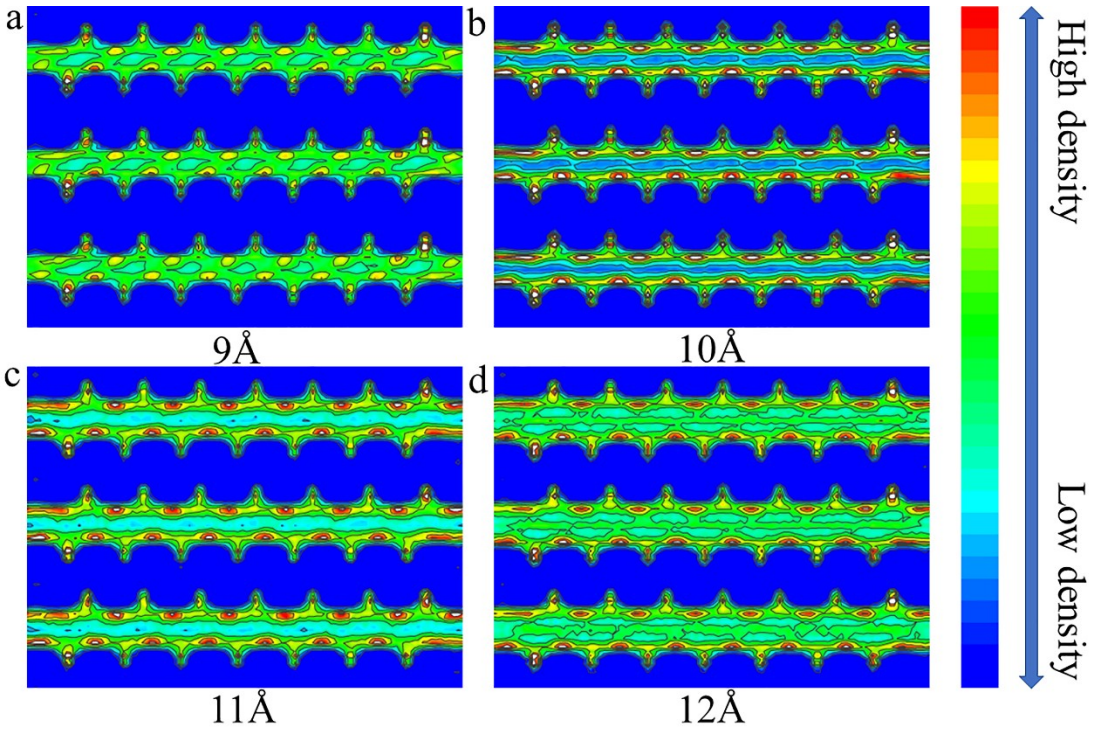

Figure S4. Water density distribution map in boridene nanochannels in four different layer spacings under the same pressure of 100MPa. These maps were projected the waters inside the channels onto the 2D plane of x-y.

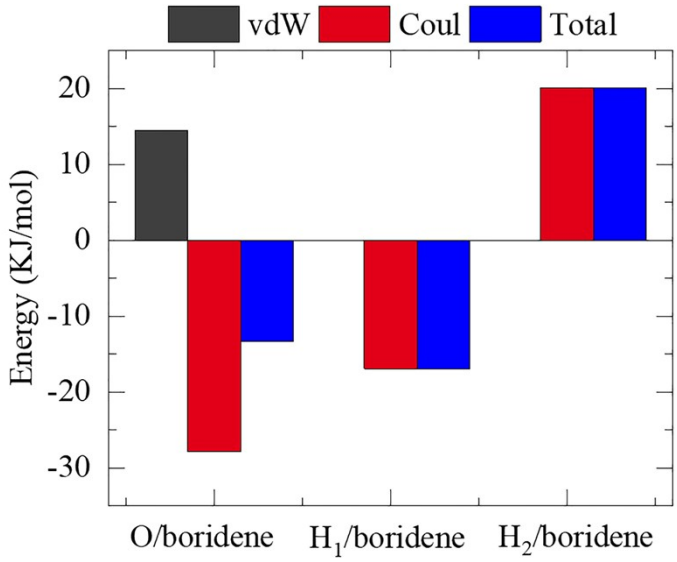

Figure S5. Interaction energies, including van der Waals (vdW), coulombic (Coul) and total energies, between boridene and atoms of water molecule adsorbed inside the groove. The O/birodene, H_1/boridene and H_2/boridene indicate the interaction between oxygen of water/hydrogen embedded into the groove/the other hydrogen over the birodene surface and

boridene, respectively. These interactions are calculated based on the structure as shown in Figure S3b.

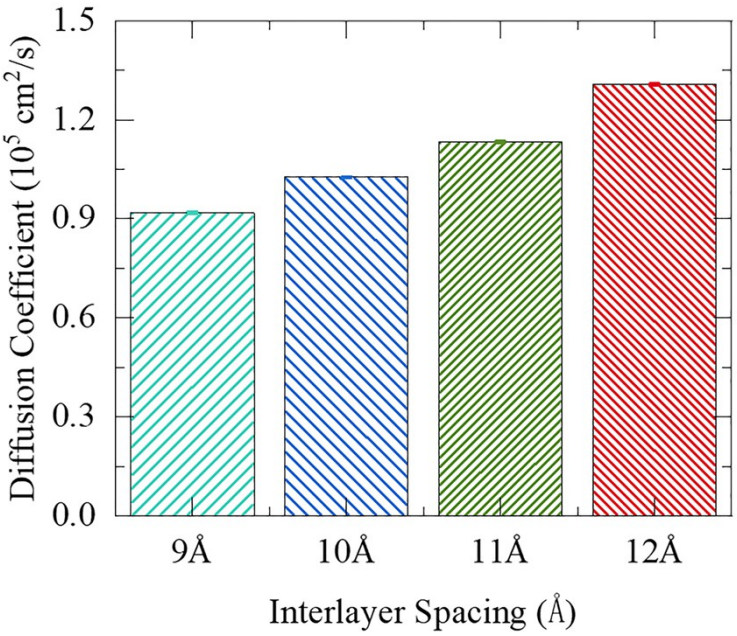

Figure S6. Diffusion coefficient of water molecules in boridene nanochannels with 4 different layer spacings. The data are obtained from three parallel trajectories under 100 MPa.

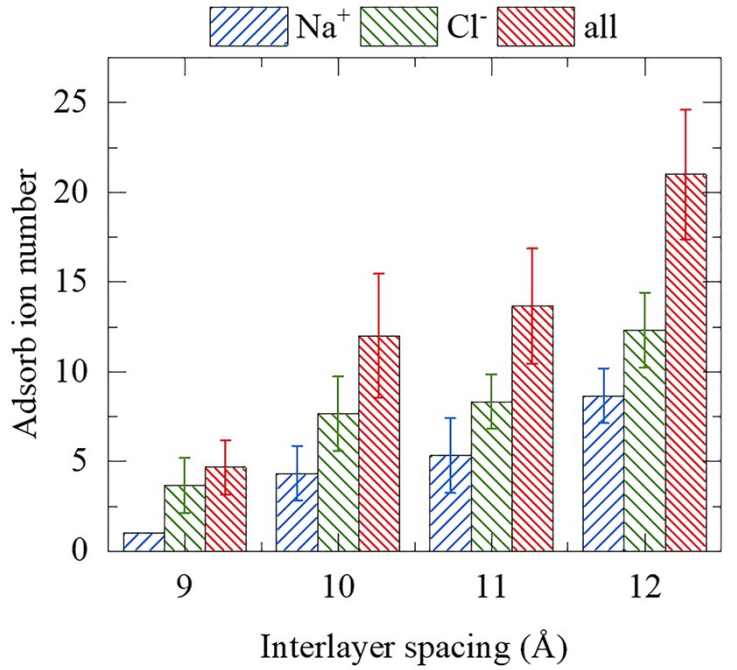

Figure S7. The number of sodium ions, chloride ions and the total number of ions adsorbed inside the boridene nanochannels at four different interlayer spacings. The data are obtained from three parallel trajectories at 100 MPa.

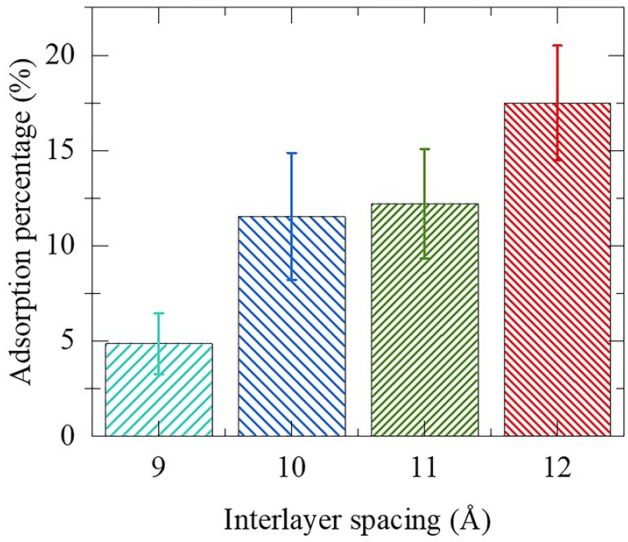

Figure S8. The rate of adsorbed ions compared with the total ions in different systems. The data are obtained from three parallel trajectories under 100 MPa

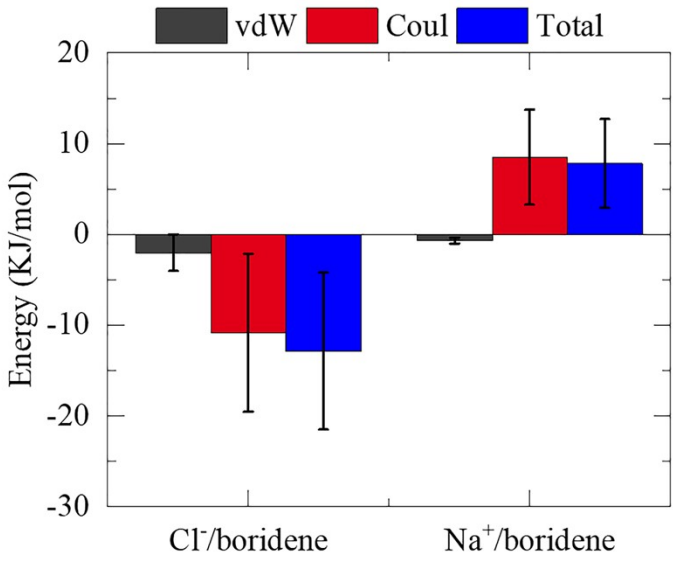

Figure S9. Interaction energy between boridene and sodium/chloride ions in the system of 12 Å interlayer spacing.

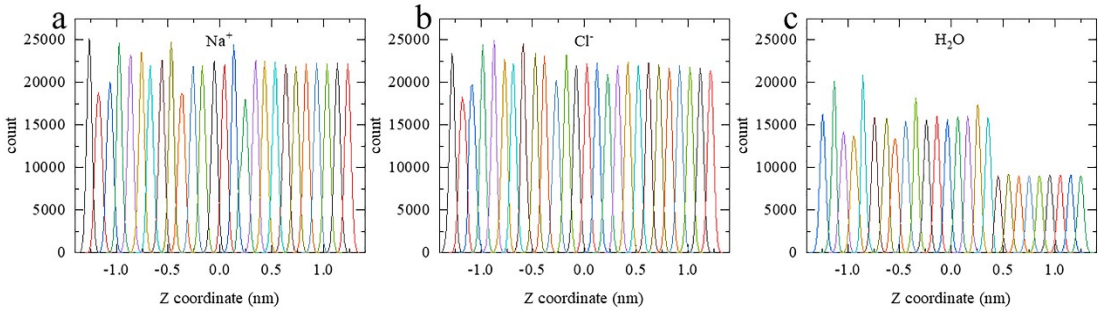

Figure S10. The sampling window histograms of PMF calculations.