Supporting Information

Why Single-layer MoS_2 is a More Energy Efficient Membrane for Water Desalination?

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Table of contents

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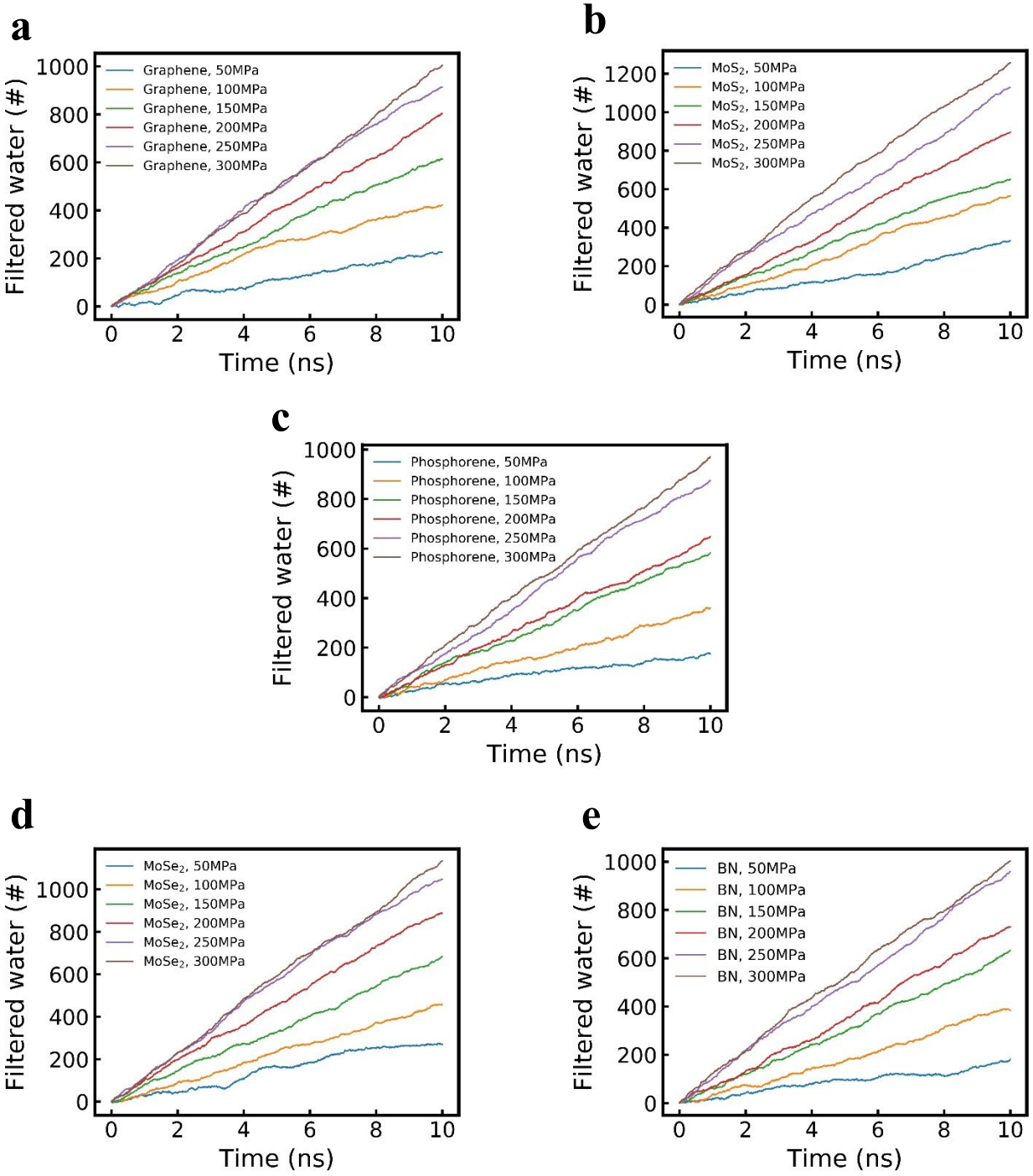
Supporting Figure 1 – Number of filtered water molecules with respect to simulation time for different material membranes | Every 5 picoseconds, the number of filtered water molecules is recorded. The slope of the filtered water vs. time is the water flux of desalination. Each graph shows the result for a single run of simulation. In this work, water flux value is calculated by taking the average of four runs with different initialization (average of the slope of four runs).



Supporting Figure 1. Number of filtered water molecules as a function of simulation time for a| Graphene membrane **b|** MoS_2 membrane **c|** Phosphorene membrane **d|** $MoSe_2$ membrane **e|** BN membrane

Supporting Table 1 | The 12-6 Lennard-Jones parameters used in simulations

Interaction	σ (Å)	ε (kcal mol^{-1})
C-C[1]	3.3900	0.0692
Mo-Mo[2]	4.2000	0.0135
S-S[2]	3.1300	0.4612
Se-Se[4]	3.2500	0.6572
P-P[5]	3.4380	0.36759
B-B[6]	3.453	0.09491
N-N[6]	3.365	0.14484
O-O[1]	0.1554	3.1656
H-H[1]	0.0000	0.0000
K-K[3]	0.4297	2.8384
Cl-Cl[3]	0.0128	4.8305
Rest	Obtained by Lorentz-Berthelot rules	

Supporting Table 2 | Pore size of different materials and pore size calculation [7]

Atoms at the edge of the pore are represented by circles. The radius of each circle is determined by the Van der Waals radius of the corresponding type of atom. The pore size is the empty area surrounded by the sketch of atom circles. Unnecessary edges are trimmed before the surrounded area is extruded. Once the extruded surface is created, final area of the nanopore can be calculated with the measuring tool of Solidworks.

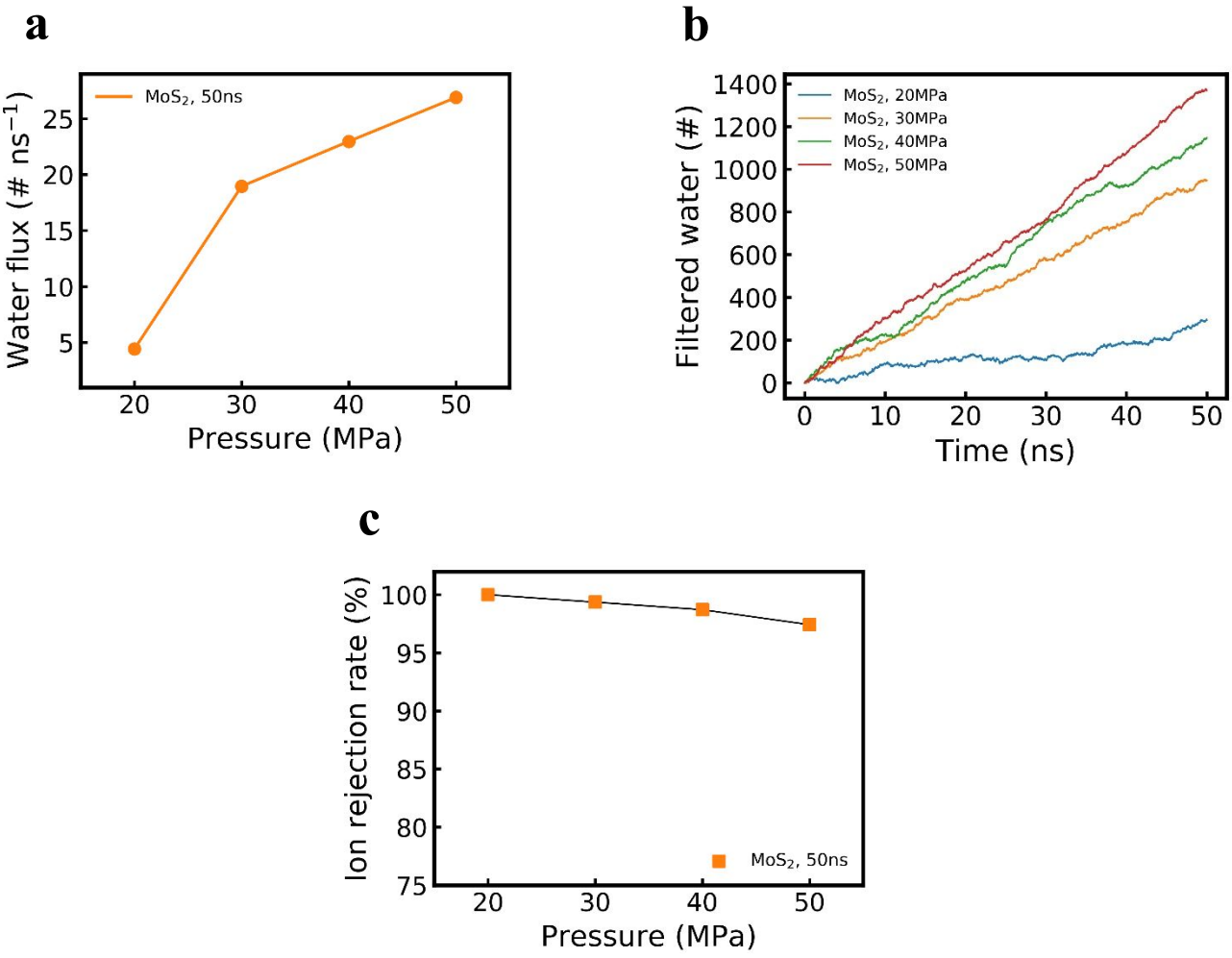
Material	Pore size (Å^2)
Graphene	49.7
MoS_2	49.6
Phosphorene	50.6
BN	49.6
$MoSe_2$	49.5

Supporting Table 3 | Exact simulation box size and number of atoms in system

The exact simulation system size varies by very small amount depending on the membrane material to accommodate the periodic boundary conditions. The exact number of atoms in system varies due to different number of atoms contained in membrane of each material.

Material	Exact box size, x, y and z (nm)	Number of atoms
Graphene	4.1753 × 4.254 × 13	15208
MoS_2	4.1 × 4.2 × 13	15171
Phosphorene	4.3077 × 4.3762 × 13	15130
BN	4.2711 × 4.3516 × 13	15282
$MoSe_2$	4.1 × 4.2 × 13	15171

Supporting Figure 2 – 50ns MoS_2 simulations with lower pressure | In practical water desalination applications, the external pressure applied should be lower than pressures simulated (50 MPa – 300 MPa), and the running time should be longer than simulated (10 ns). Therefore, in order to conduct a more thorough study on cases with lower pressure and longer running time, simulations were run with 20 MPa – 50 MPa external pressure for 50 ns to show the performance of MoS_2 in terms of water flux as well as ion rejection. At a longer time span as 50 ns, the flux we calculated was the same as calculated for 10 ns simulations and the ion rejection rates still maintained over 97%.

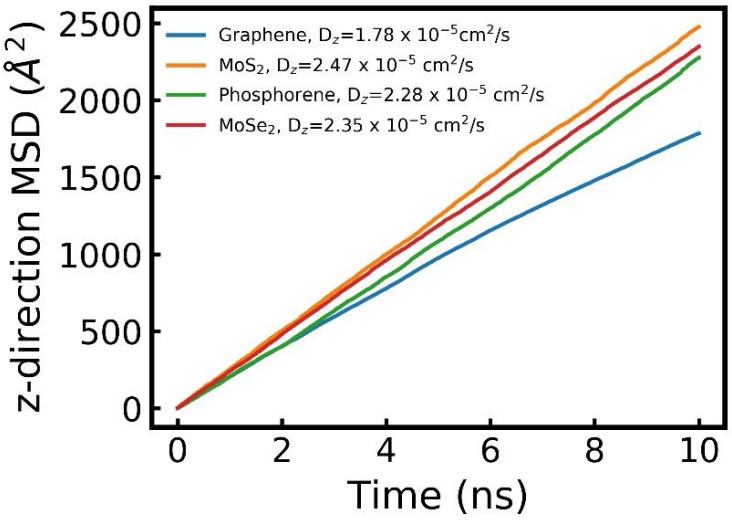


Supporting Figure 2a| Water flux of MoS_2 under pressures ranging from 20 MPa – 50 MPa in 50 ns simulations **b|** Number of filtered water molecules with respect to time under pressures ranging from 20 MPa – 50 MPa in 50 ns MoS_2 simulations **c|** Ion rejection rate of MoS_2 under pressures ranging from 20 MPa – 50 MPa in 50 ns simulations

Supporting Figure 3 – Mean squared displacement and diffusion coefficient of water near membranes | The *z*-direction MSD data were collected for water molecules in a bin which had the size of 4 nm × 4 nm × 0.2 nm and was positioned at 0.2 nm away from membrane in the saline water section. The diffusion coefficient of water in z-direction (denoted as *Dz*) can be calculated from MSD of center of mass of water molecules using the equation:[1]

$$\langle |(r(t) - r(0))|^2 \rangle = 2D_z t$$

where *Dz* is the diffusion coefficient; *r(t)* is the direction position of water molecules; and *t* is the time. *Dz* for MoS_2, Phosphorene, Graphene and $MoSe_2$ were calculated to be 2.51 × 10^{-5} cm^2/s, 2.12 × 10^{-5} cm^2/s, 1.78 × 10^{-5} cm^2/s, 2.35 × 10^{-5} cm^2/s, respectively. Higher diffusion coefficient of water near MoS_2 compared with other membrane materials implies that water molecules near MoS_2 have less interfacial friction to move in *z*-direction.



Supporting Figure 3| Water mean squared displacement near membrane in saline water section. The data are collected when no pressure is applied.

Supporting References

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