

Supporting Information to

**Comparison of water desalination performance of porous graphene
and MoS₂ nanosheets**

By

Zailing Song^{#a}, Yunlong Niu^{#bc}, Juan Yang^a, Liang Chen^a, Junlang, Chen^{*a}

^aDepartment of Optical Engineering, College of Optical, Mechanical and Electrical Engineering, Zhejiang A&F University, Lin'an 311300, China

^bthe State Key Laboratory of Industry Control Technology, College of Control Science and Engineering, Hangzhou 310027, China.

^cRadiation Monitoring Technical Center of Ministry of Ecology and Environment, State Environmental Protection Key Laboratory of Radiation monitoring, Hangzhou 310012, China.

These authors contributed equally to this work.

* Corresponding author Email: chenjunlang7955@sina.com

Table S1. The 12-6 Lennard-Jones parameters used in the simulations

Interaction	$\sigma[\text{\AA}]$	$\epsilon[\text{kcal mol}^{-1}]$
S-S ¹	3.1300	0.4612
Mo-Mo ¹	4.2000	0.0135
C-C ²	3.3900	0.0692
H-H ²	0.0000	0.0000
O-O ²	3.1656	0.1554
Na-Na ³	2.1600	0.3526
Cl-Cl ³	4.8305	0.0128
C-O ⁴	3.4360	0.0850
C-H ⁴	2.6900	0.0383
Rest	Obtained by Lorentz-Berthelot rules.	

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- 3 I. S. Joung and T. E. Cheatham, *J. Phys. Chem. B*, 2008, **112**, 9020–9041.
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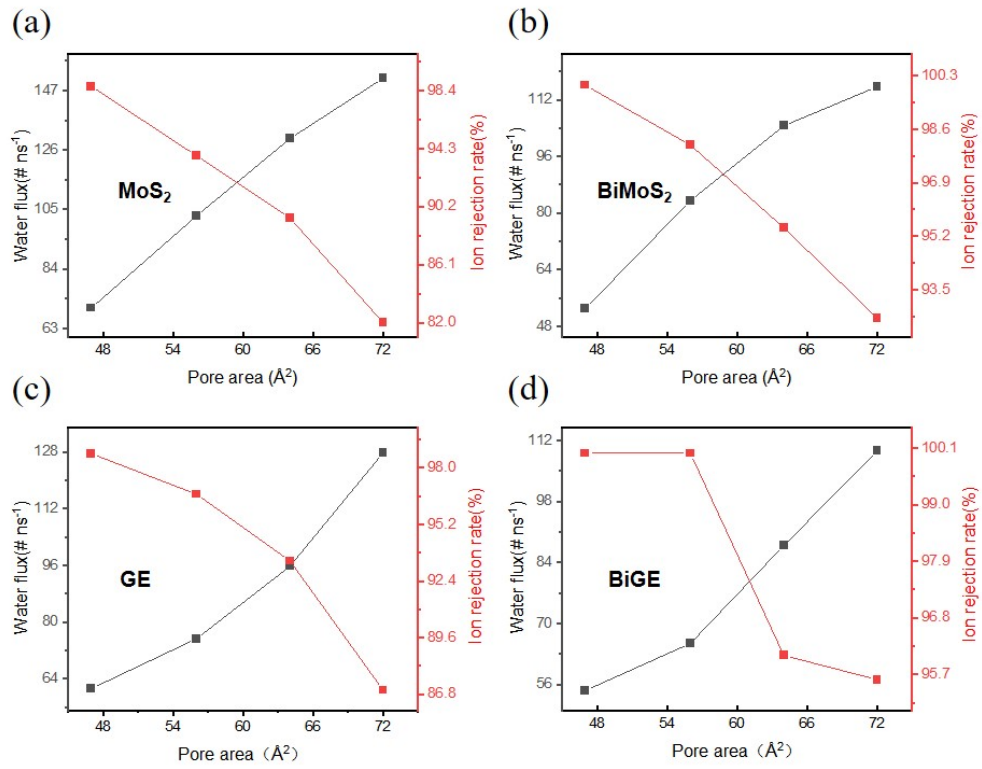


Figure S1. Water flux and ion rejection against pore size of the four membranes at 200 MPa. (a) MoS₂ monolayer, (b) MoS₂ bilayer, (c) GE monolayer, (d) GE bilayer.

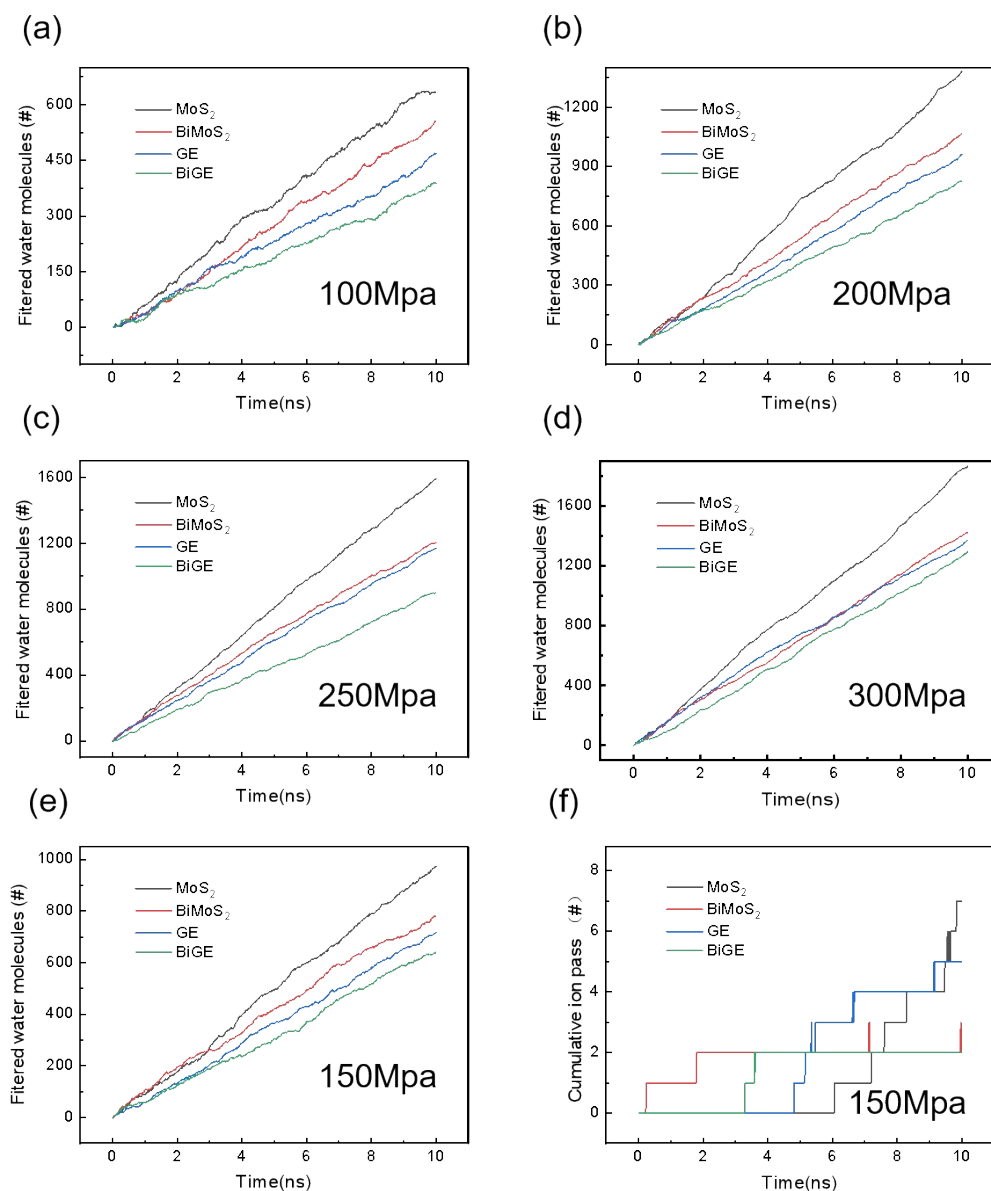


Figure S2. (a-d) The relationship between the number of filtered water molecules and the simulation time for membranes with different materials under different pressures. (e) Number of water molecules and (f) number of Na⁺ pass through the nanopore as a function of simulation time for four nanopores at a fixed pressure (150 MPa) and a fixed pore area (64 Å²).

It can be seen from Figure S2 that the water flux of MoS₂ is much larger than that of GE regardless of monolayer and bilayer under each exerted pressure. As for monolayer membrane, MoS₂ performs 19.8%, 36.8%, 35.3% and 37.4% better than GE in terms of water permeation under external pressures of 100 MPa, 200 MPa, 250

MPa and 300 MPa, respectively. Similarly, BiMoS₂ membranes perform 29.9%, 19.1%, 16.5% and 18.4% better than BiGE membranes.