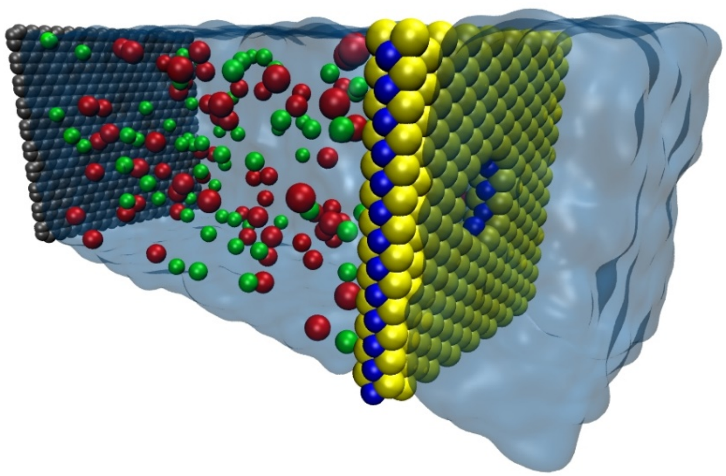
Molybdenum Disulfide as a Novel 2D Nano-porous Membrane for Water Desalination

PI: Narayana R. Aluru
Presenter: Mohammad Heiranian

Department of Mechanical Science and Engineering,
Beckman Institute for Advanced Science and Technology,
University of Illinois at Urbana–Champaign

2D Materials in Desalination & DNA Sequencing

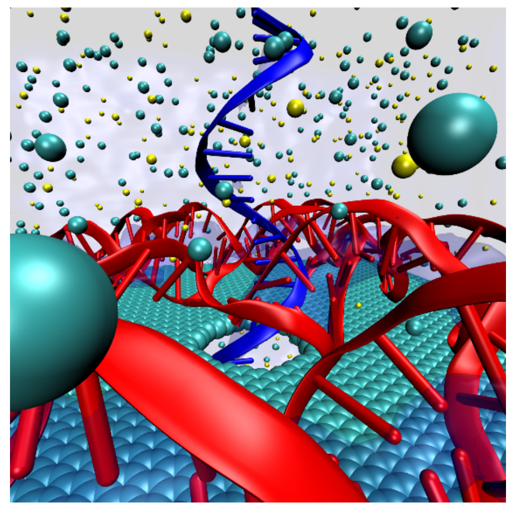
Desalination using Molybdenum disulfide (MoS2)



High water flow rates while rejecting ions effectively

(Nature Commutations 2015, N. R. Aluru)

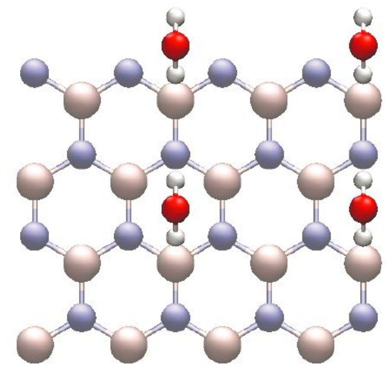
DNA base detection using hybrid graphene-DNA origami pores

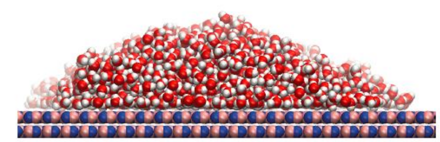


Origami nanopore retards DNA translocation speed improving the single resolution

(ACS Nano, under review, N. R. Aluru)

Hexagonal boron nitride-water interaction using quantum Monte Carlo





Force field development for the interaction between water and hBN

(Journal of Chemical Physics 2015 , N. R. Aluru)

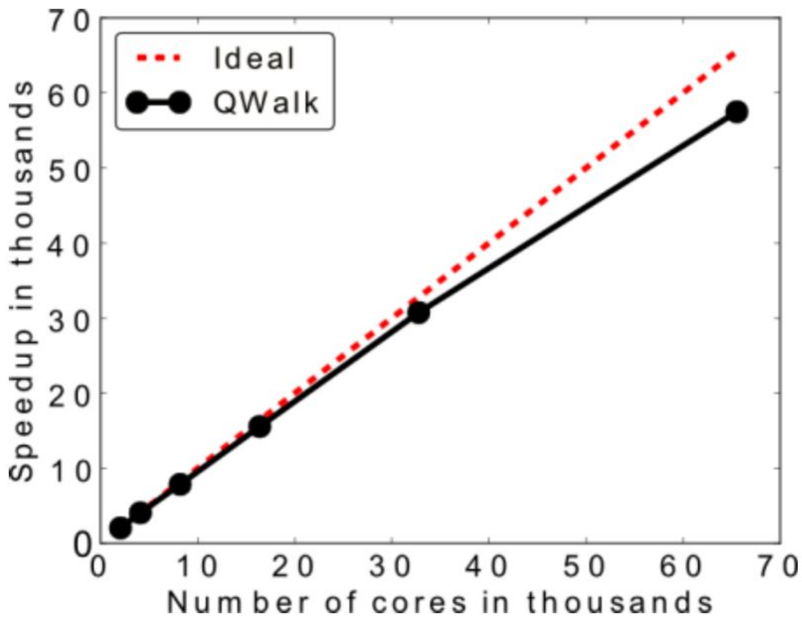
Using the Power of Blue Waters

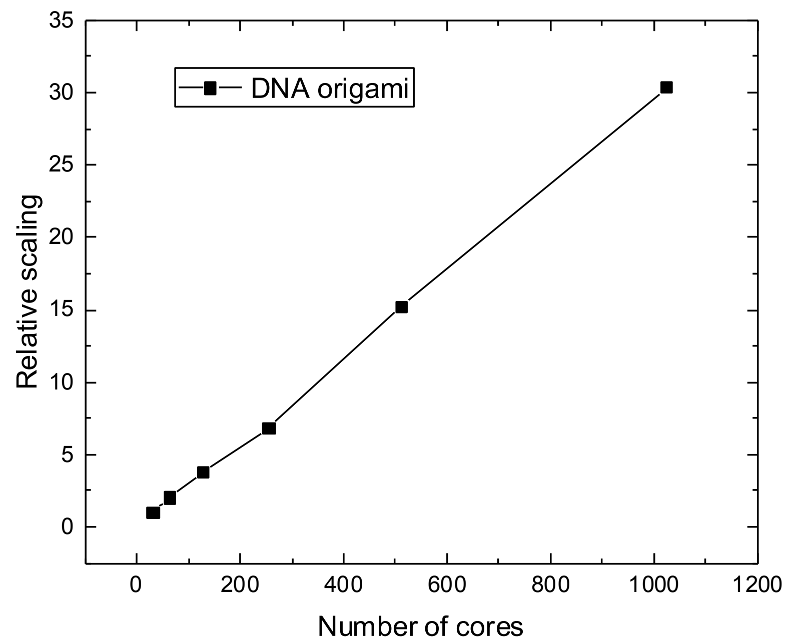
- BW nodes have sufficiently high memory of 64 GB per node (A Stampede node has 32 GB)
- BW nodes have a high peak memory of GB/s
- Efficient for calculations requiring reading and writing large amount of data

Node	Peak Memory GB/s
Blue Water Cray XE	102
NICS Kraken Cray XT	25.6
NERSC Hopper XE	85.3
ANL IBM BG/Q	42.6

Using the Power of Blue Waters

Scaling of QWalk and NAMD on Blue Waters

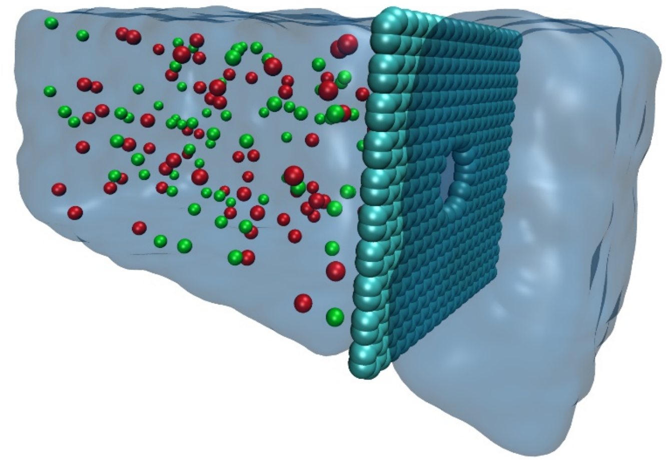


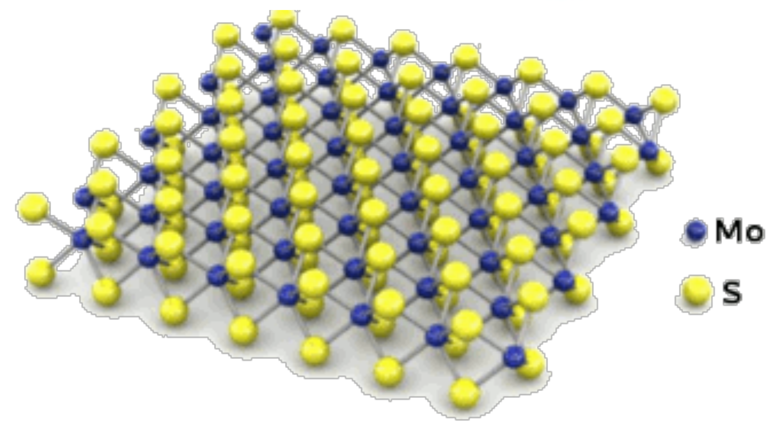


Water desalination, DNA origami sequencing and Monte Carlo calculations cost ~150,000, ~300,000 and ~275,000 node hours on Blue Waters

Water Desalination: Introduction & Motivation

* Permeation rate is one of challenges in reverse osmosis
* Thin membranes are advantageous as flux scales inversely with thickness
* Graphene has several orders of magnitude higher permeation rate than that of existing membranes
* Adding hydroxyl groups to graphene pores (hydrophilic) enhances water permeation
* MoS_2 : two types of atoms with thickness of about 1 nm
* It is mechanically robust with Young's modulus (270 +/- 100 GPa)
* MoS_2 was shown to provide better results in DNA sequencing compared to graphene





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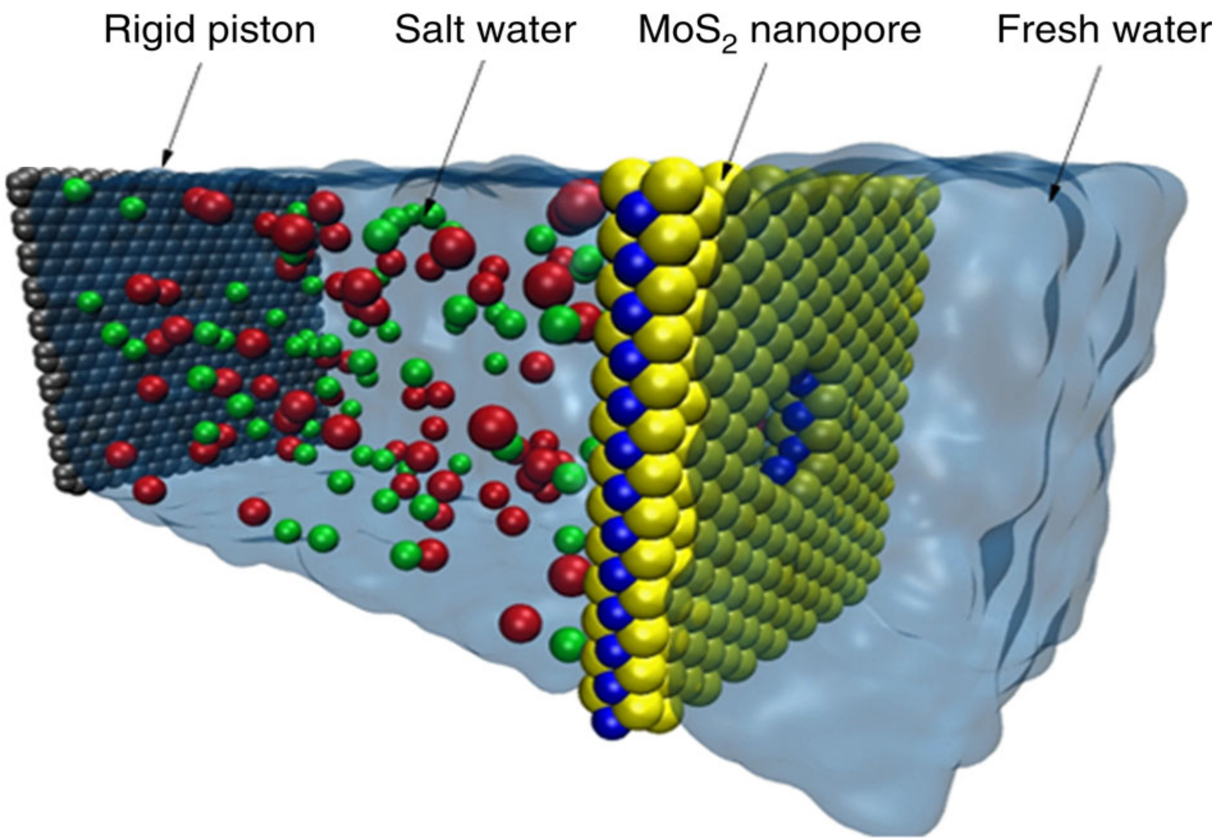
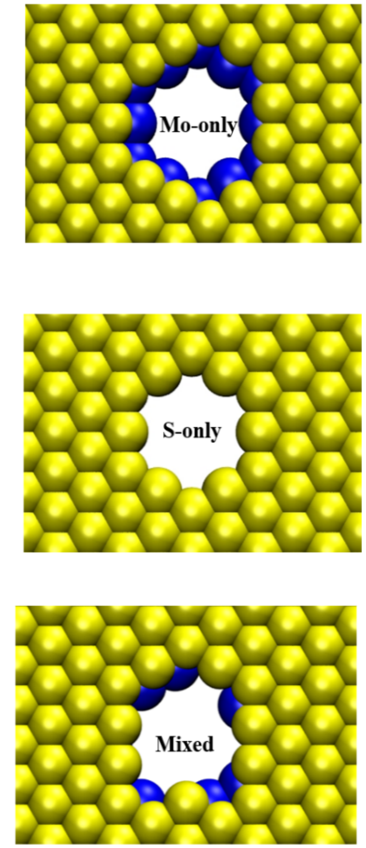
Cohen-Tanugi, D. & Grossman, J. C. Nano Lett. 12, 3602–3608 (2012).
Feng, J. et al. Nano Lett. 15, 3431–3438 (2015).
Farimani, A. B., Min, K. & Aluru, N. R. ACS Nano 8, 7914–7922 (2014).

Method



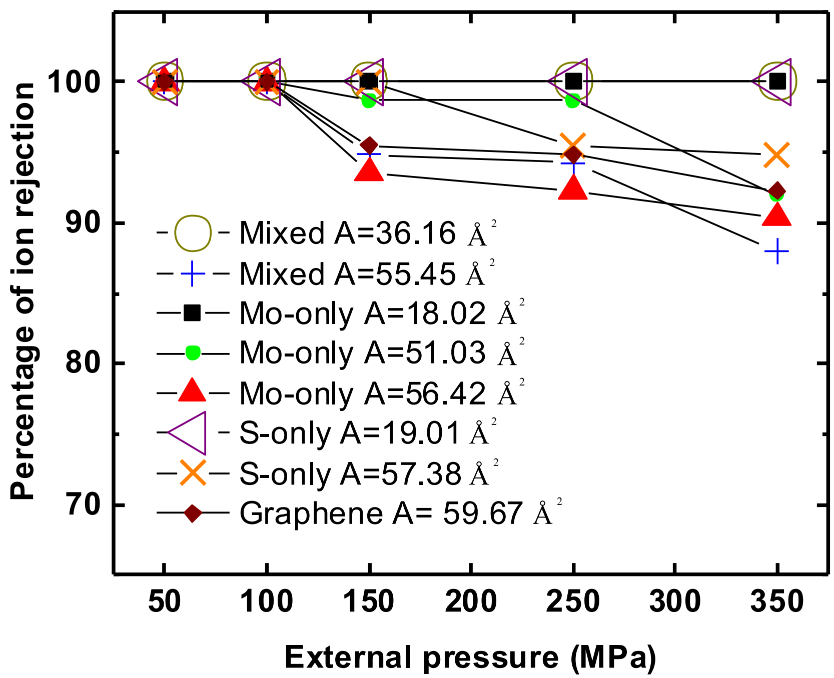


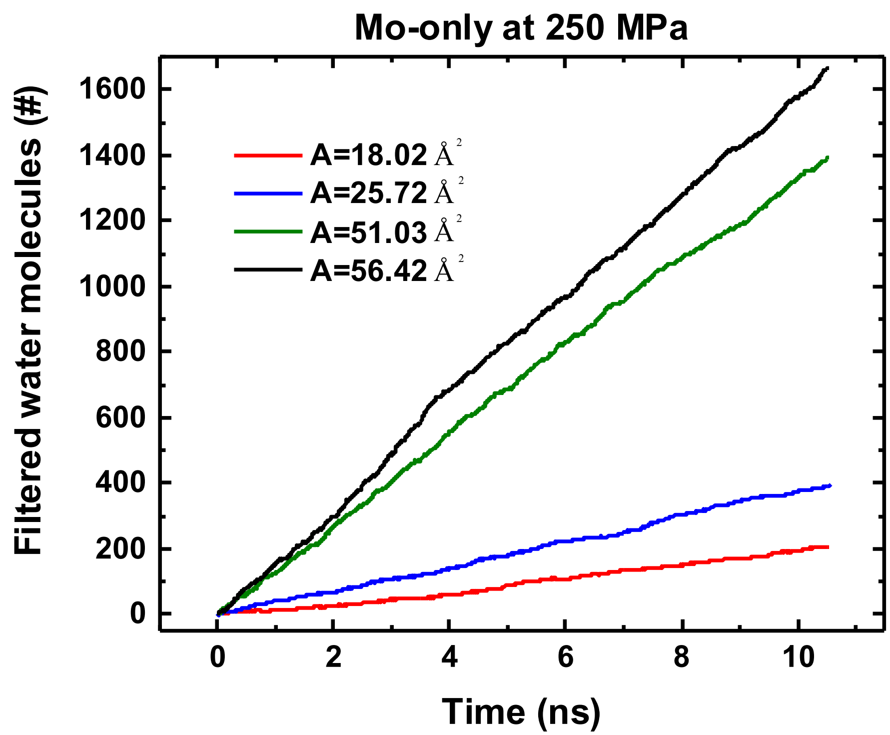
* 3 types of pores with sizes ranging from 20 to 60 $Å^2$
* 1 molar of salt (seawater, 0.599 M)
* Molecular dynamics simulations
* Force-field developed by Liang *et al*. used for MoS2

Liang, T., Phillpot, S. R. & Sinnott, S. B. Phys. Rev. B 79, 245110 (2009)

Results: Rejection & Pore Sizes

- Ion rejection of small pores is 100% for all types of pores
- For larger pores, ions escape through the pore reducing rejection efficiency
- Water rate increases sharply as pore area increases from ~20 to ~50 Å^2 (single-file water in small pores)



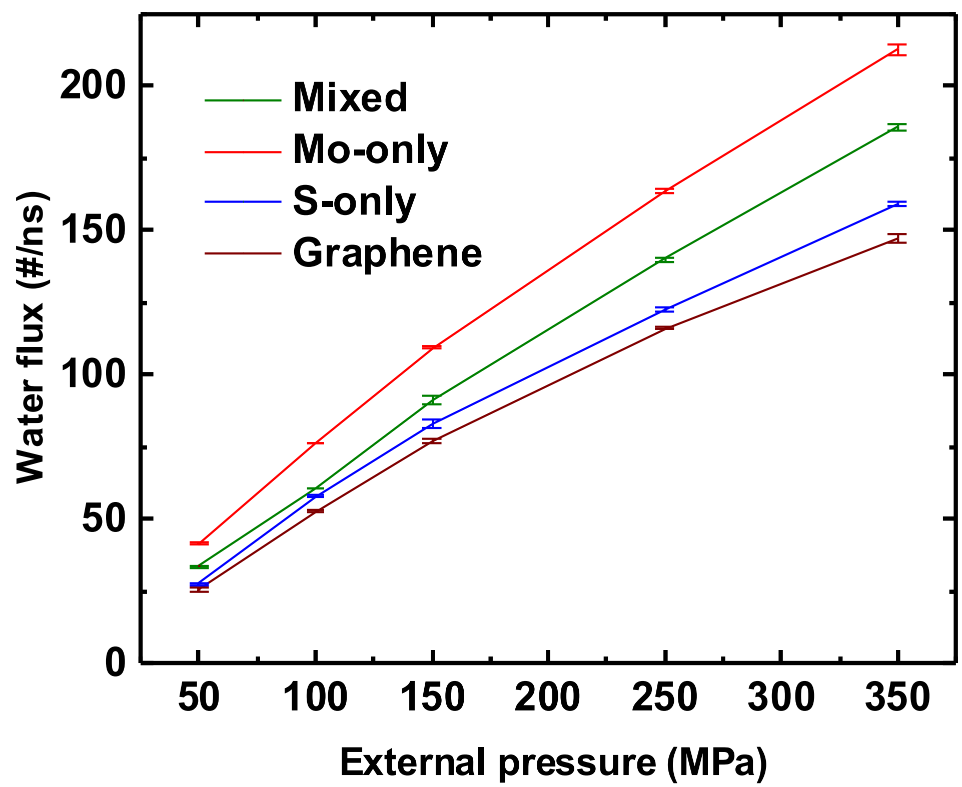


Results: Permeation Rate

* Water flux as a function of applied pressure

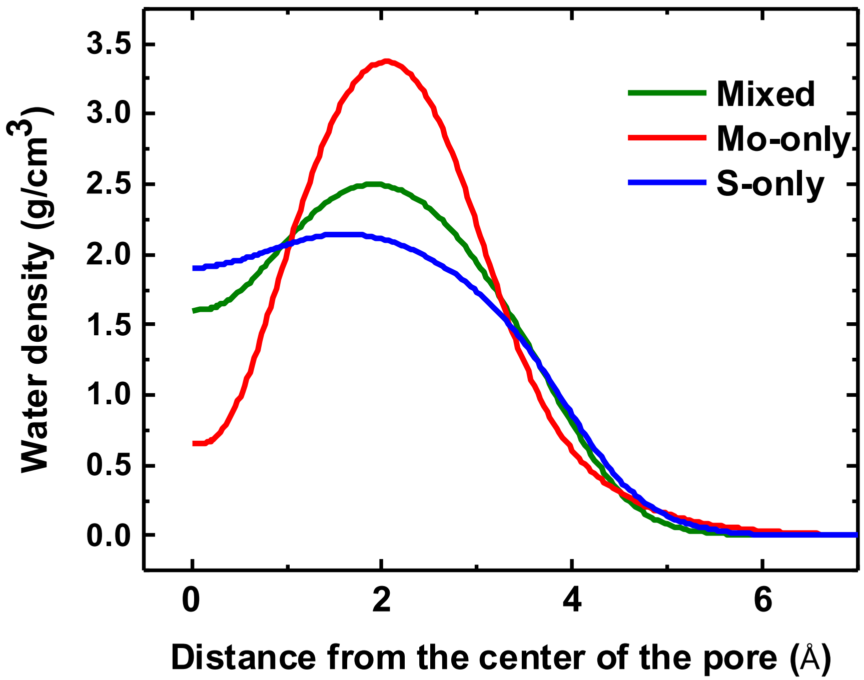
* Similar pore areas: Mixed 55.45 , Mo-only 56.42 , S-only 57.38 and graphene 59.67 $Å^2$

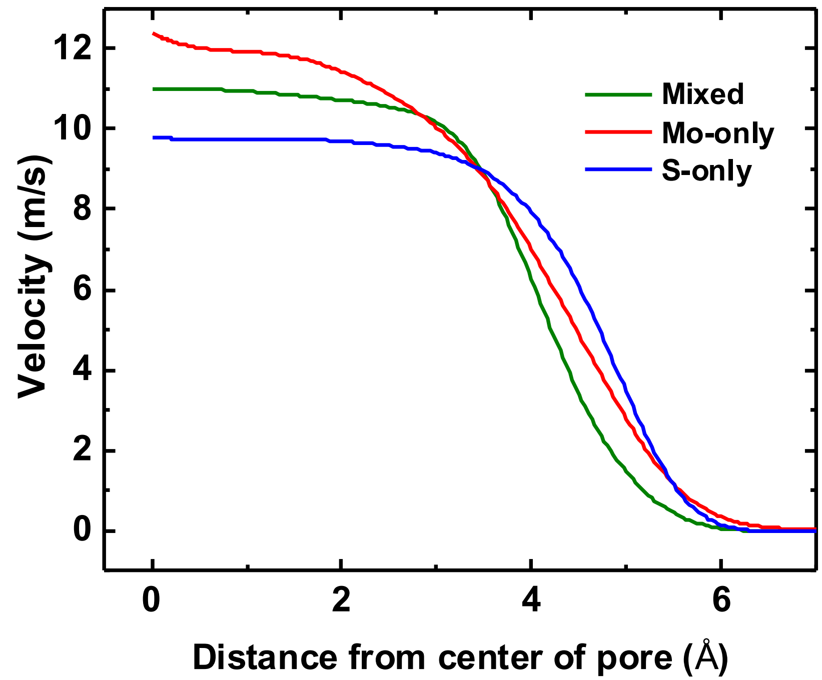
* Mo-only has highest rate of permeation followed by Mixed, S-only and graphene pores



Results: Density & Velocity

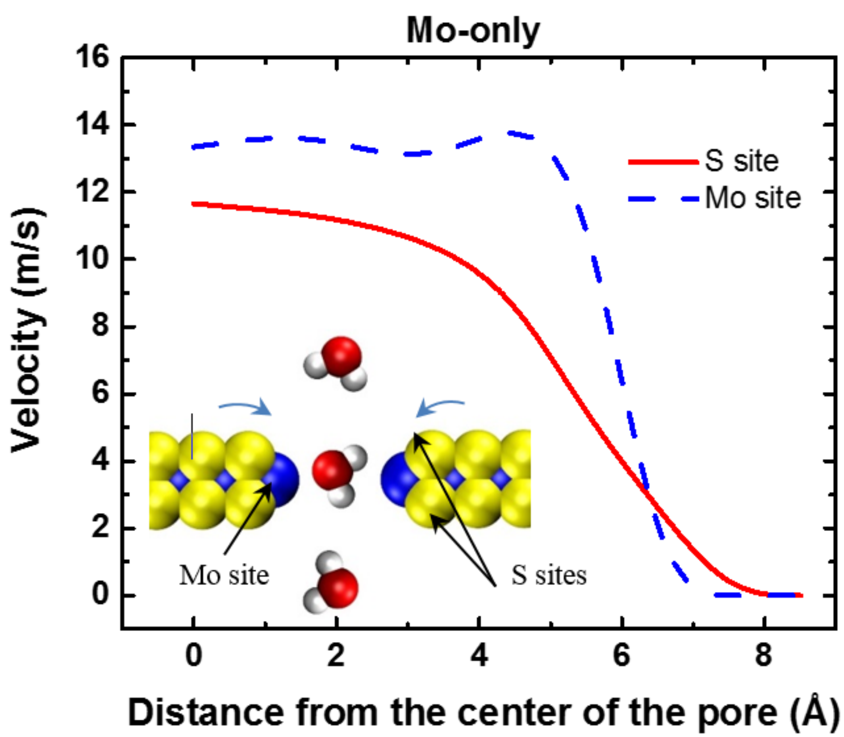
* High rates in Mo-only pore is explained by higher water density and velocity
* Higher density in Mo-only pore can be attributed to hydrophilic nature of Mo
* Average density of water follows order of Mo-only>Mixed> S-only (1.47, 1.37 and 1.31 g/cm3)
* Average velocity of water is 8.26, 7.53 and 7.51 m/s

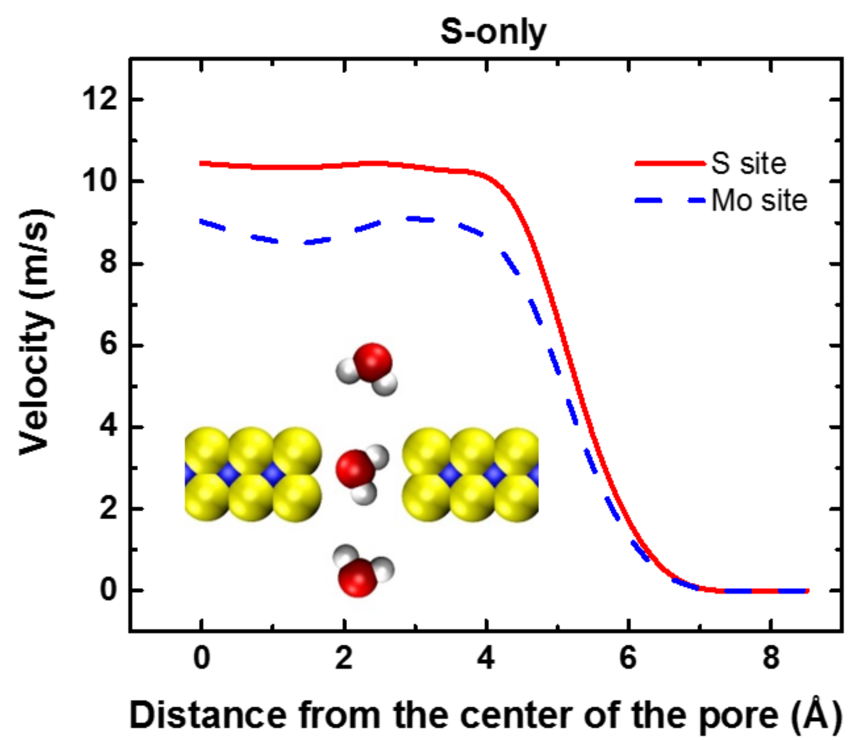




Results: Velocity

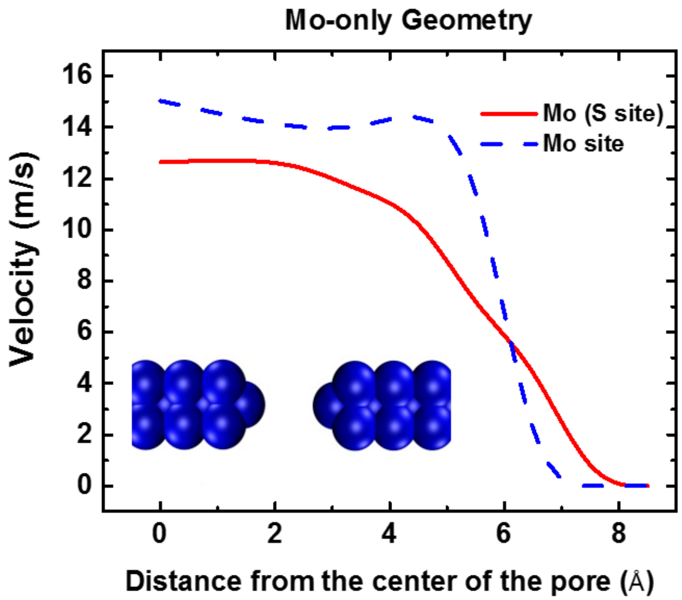
* Velocity profiles at sites of S and Mo
* In Mo-only pore, velocity is higher at Mo. Velocities are higher in S site in S-only pore
* Arrangement of Mo and S sites and geometry of pore matter in velocities

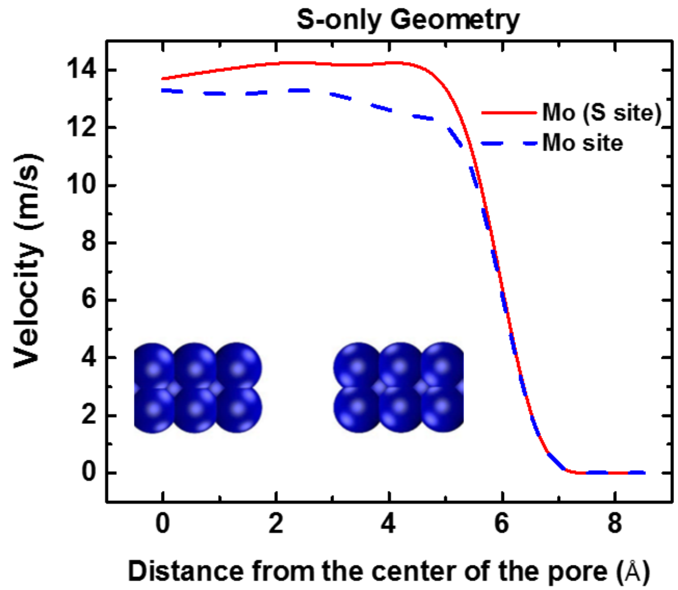




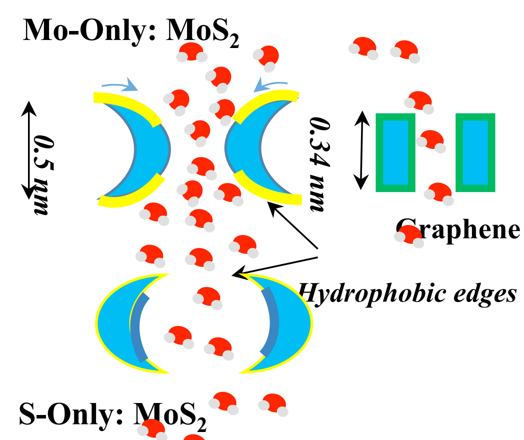
Results: Velocity

* All atoms Mo with same geometry: shapes of velocity profiles are identical





* Conical nanopores have higher fluxes and permeation rates (aquaporin, solid-state nanopores)
* Mo-only has a conical nanopore giving rise to higher fluxes



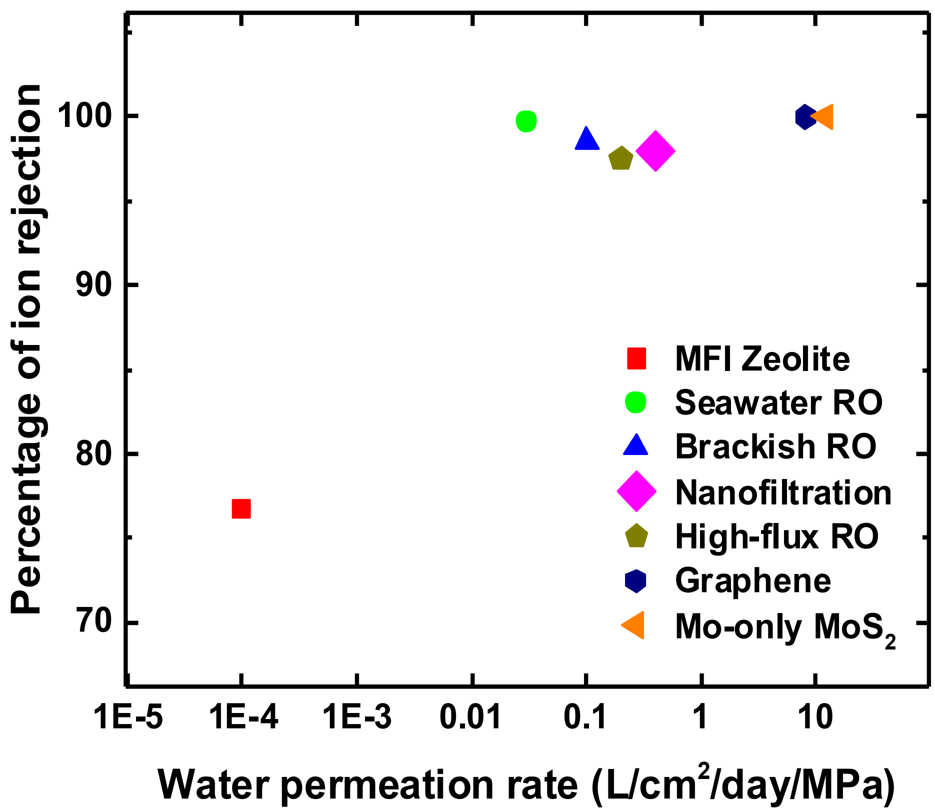
Gravelle, S., Joly, L., Ybert, C. & Bocquet, L. *J. Chem. Phys.* **141**, 18C526 (2014).
Farimani, A. B., Aluru, N. R. & Tajkhorshid, E. *Appl. Phys. Lett.* **105**, 83702–83702(2014).

Discussion

* Ion rejection and water flux are two important factors defining effectiveness and performance

* Permeation rate is theoretically enhanced by 5 orders of magnitude compared to MFI-type zeolite

* There is a 70% improvement in permeation rate compared to graphene



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Conclusions & Acknowledgment

* MoS_2 membranes are promising for water purification and salt rejection
* Conical architecture of Mo-only pore with special arrangement of hydrophobic edges and hydrophilic center enhances water permeation
* Water permeation rates associated with these MoS_2 membranes are found to be 2 to 5 orders of magnitude greater than that of currently used membrane materials and 70% better than graphene nanopore

Special thanks to Blue Waters for making this possible!

Thanks for your attention!

Questions?