Single-layer MoS_2 Nanopores as Power Generators

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

Using the Power of Blue Waters

* BW nodes have sufficiently high memory of 64 GB per node (A Stampede node has 32 GB)
* 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

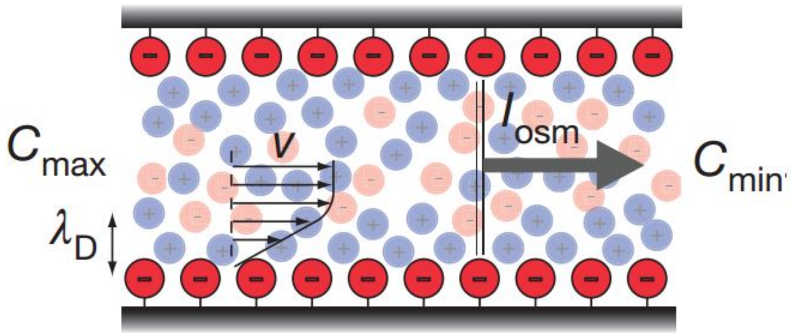
Introduction & Background

* Power can be generated from salt concentration gradients (e.g. seawater & river)
* Charged nanoporous membranres are selective to counter ions
* Because of the selectivity, more counter ions diffuse down the gradient

Corresponding diffusion potential

$$V_{diff} = S(\Sigma)_{is} \frac{RT}{F} \ln\left[\frac{a_{KCl}^{cis}}{a_{KCl}^{trans}}\right]$$

Selectivity factor

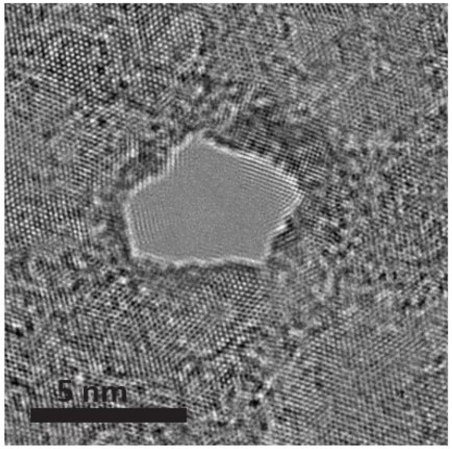


Siria, Alessandro, et al. Nature (2013).

Experimentally, a boron nitride nanotubve was shown to generated large electric currents

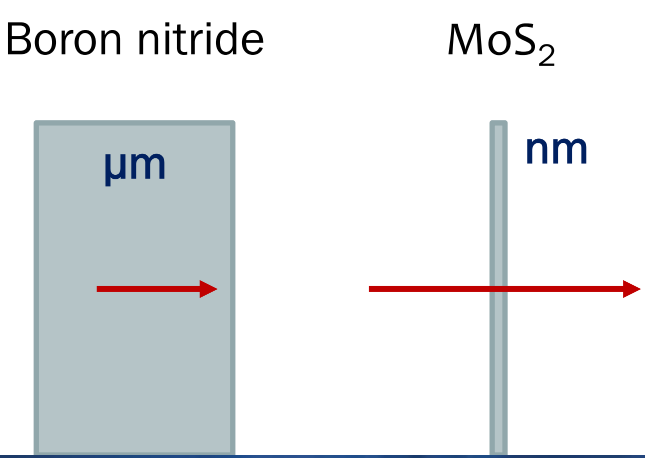
Introduction & Background

* 2D membranes are ideal as the thinness leads to higher transport rates
* MoS_2 :
    1. Thickness of less than 1 nm
    2. Selective pore charge density ranging from -1 to -9 e/nm^2 depending on pH
* With the few-atom thick membrane, a stronger power generation is expected



A MoS_2 nanopore in the experiment

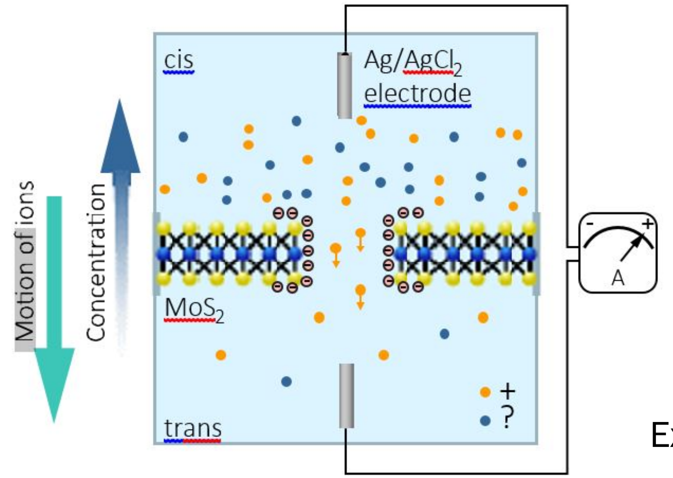
Membrane	Power density (W/m^2)	Membrane thickness
Weinstrin and Leitz, 1976	0.17	1 mm
Audinos, 1983	0.40	3 mm
Turek and Bandura, 2007	0.46	0.19 mm
Suda et al, 2007	0.26	1 mm
Veerman et al, 2009	0.95	0.2 mm
Kim et al, 2010	7.7	0.14 mm
Siria et al, 2013	4000	1um
This work	?	0.65 nm



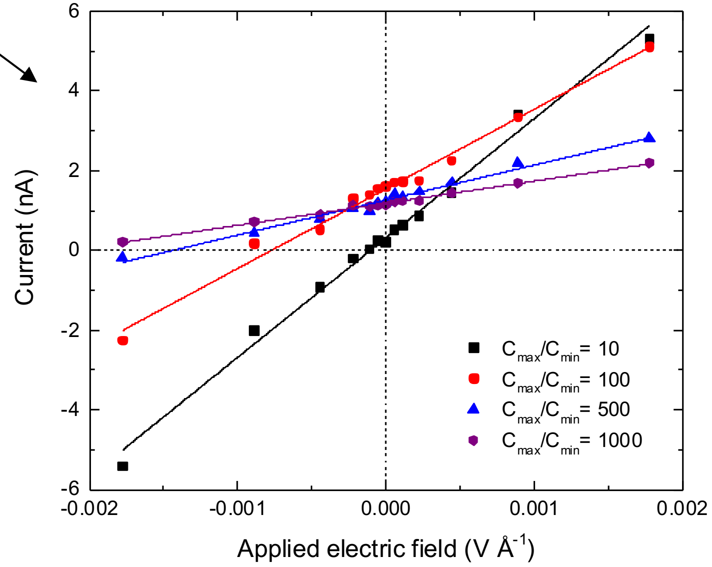
Results: Current & Voltage

* Different salinity ratios of 10, 100, 500 and 1000 of KCl in MD simulations

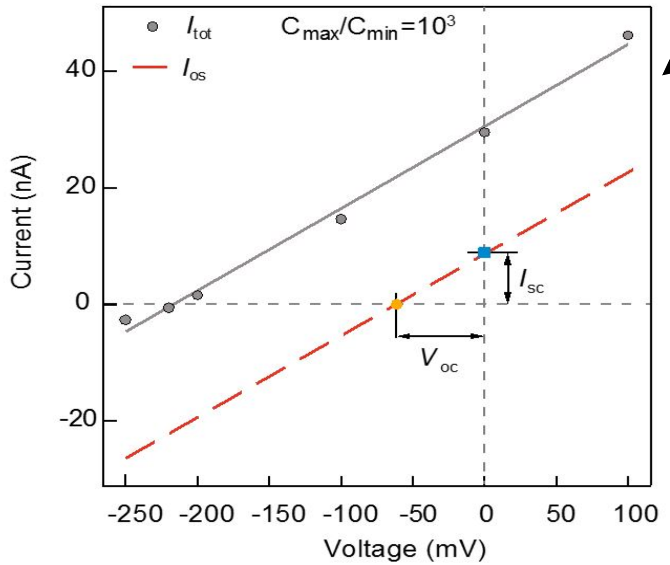
* Short circuit current and open circuit voltage are characteristics of a power generator in porous membranes



MD



Experiment

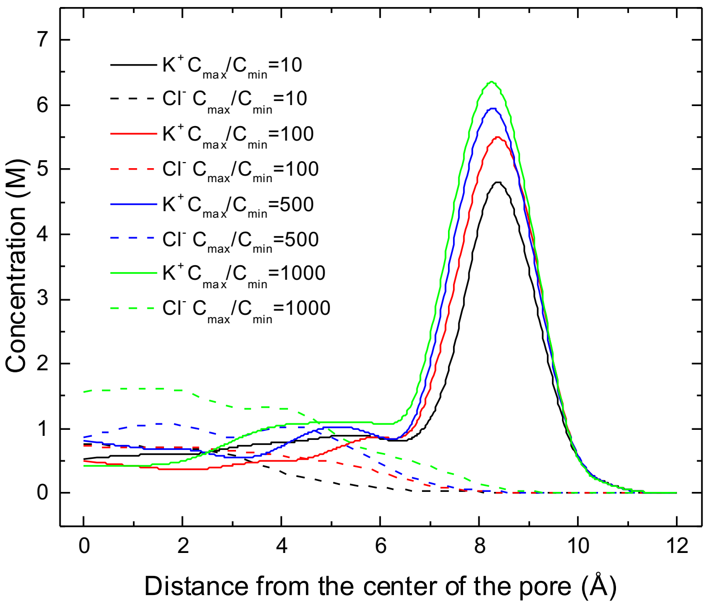


Results: Selectivity

- Flux of each ion depends on its concentration and velocity inside the pore
- Potassium ions are attracted to the charged surface of the pore
- A double layer near the surface
- Selectivity decreases with concentration ratio

Potassium selectivity $\longrightarrow$ $$\frac{J_{K^+} - J_{Cl^-}}{J_{K^+} + J_{Cl^-}}$$

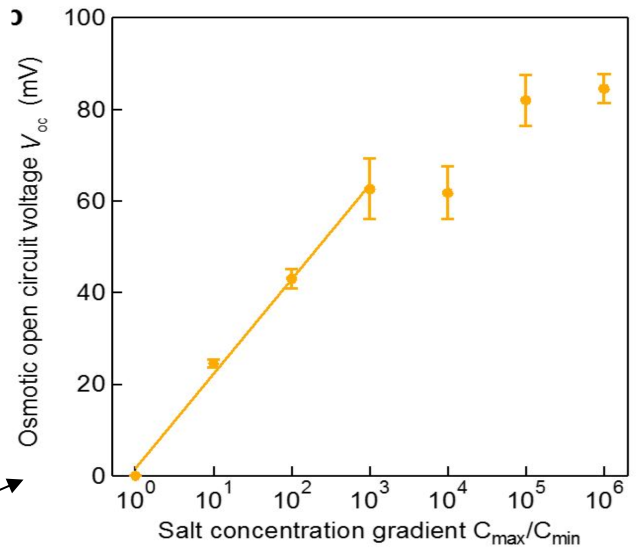
Concentration ratio	J_{K^+} [#/ns]	J_{Cl^-} [#/ns]	Potassium selectivity coefficient
10	2.34	0.34	0.7462
100	15.34	2.67	0.7034
500	12.67	2.34	0.6882
1000	10.34	2.00	0.6758

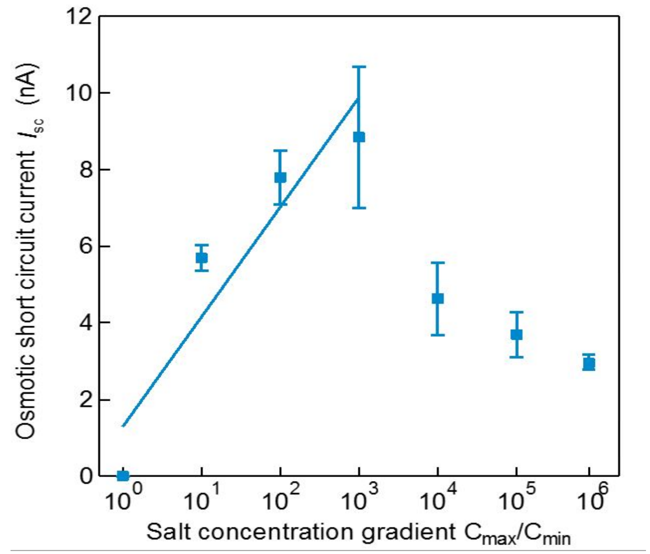


Results: Current & Voltage

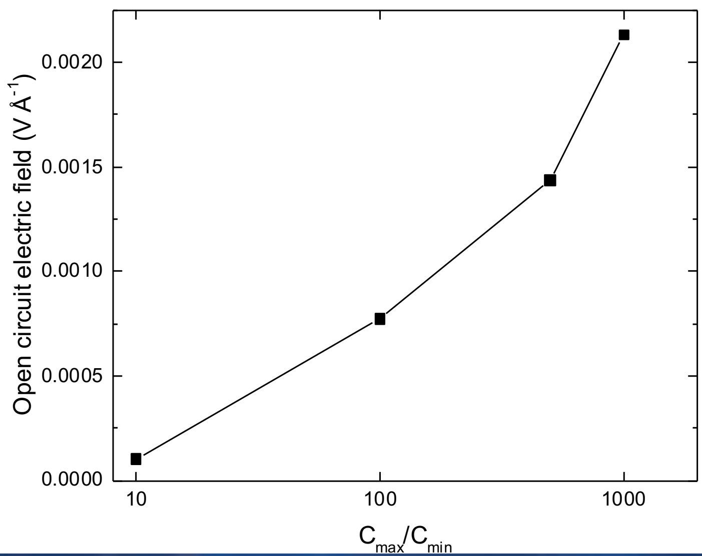
- Open circuit voltage (or electric field) increases with salinity ratio
- Non monotonic behavior for current and salinity ratio

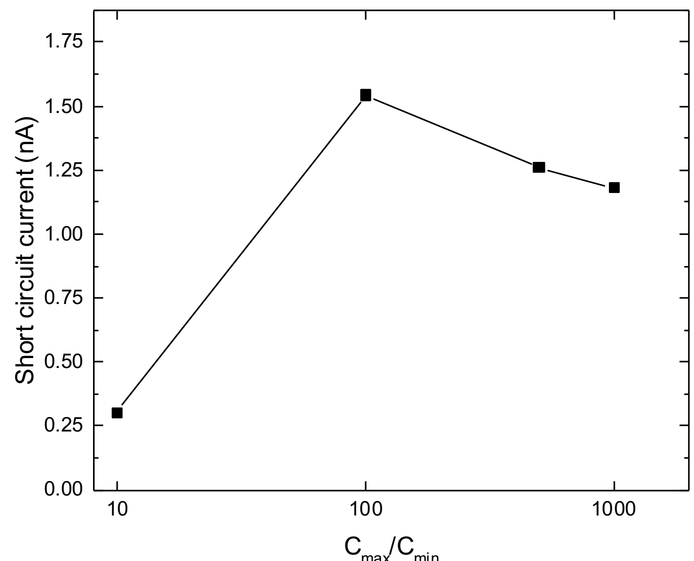
Experiment





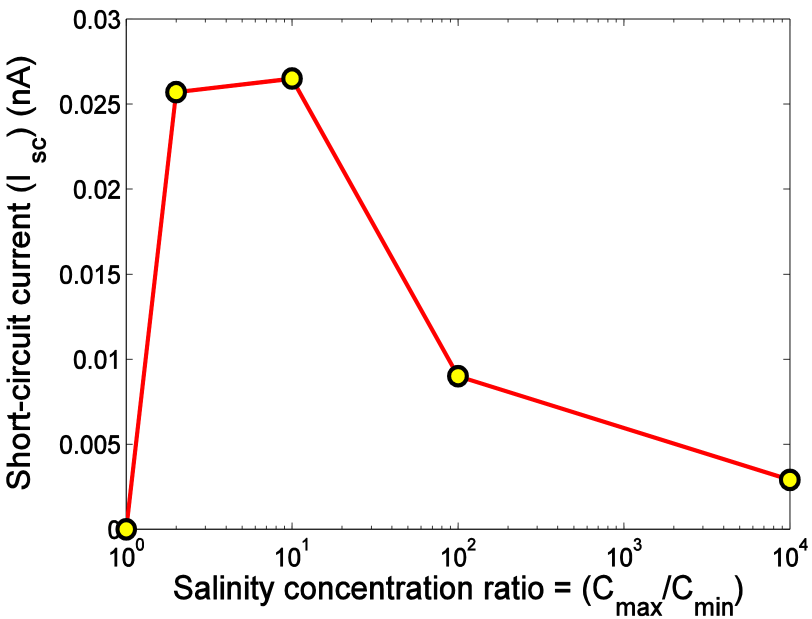
MD

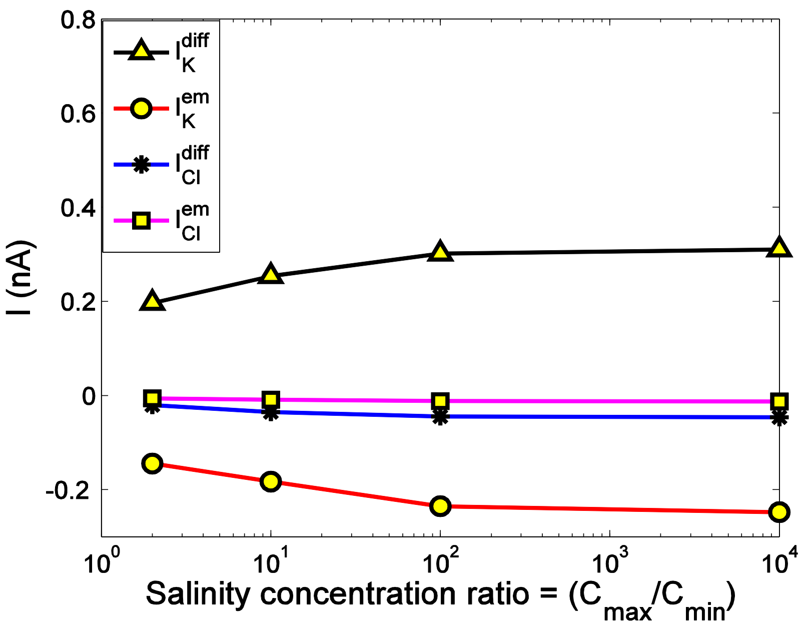




Results: Non-monotonic Current

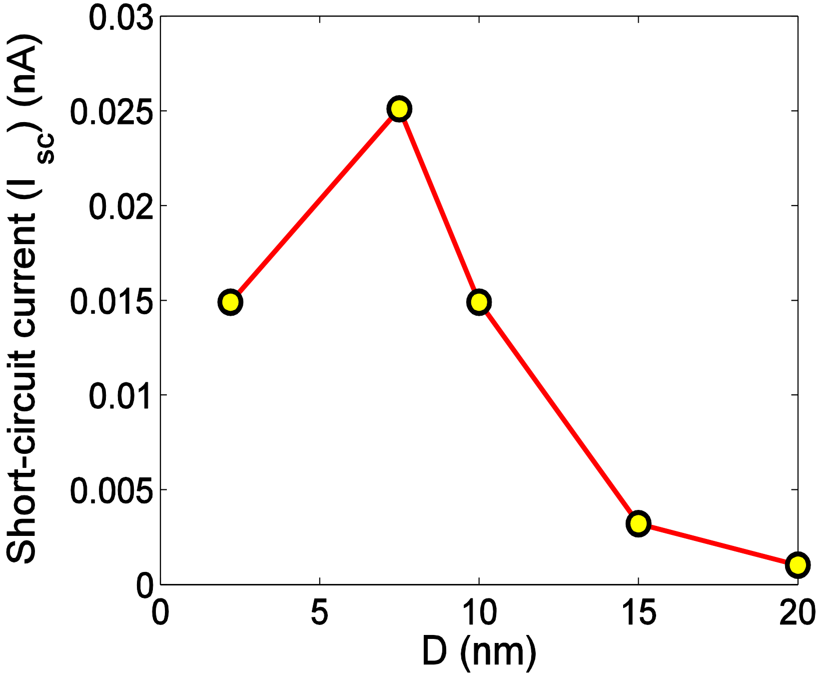
* Continuum based analysis is carried out to understand the non-monotonic behavior
* Dominant component of the current is due to diffusion and migration of ions
* At high salinity ratios, migration current starts to contribute more suppressing the total current

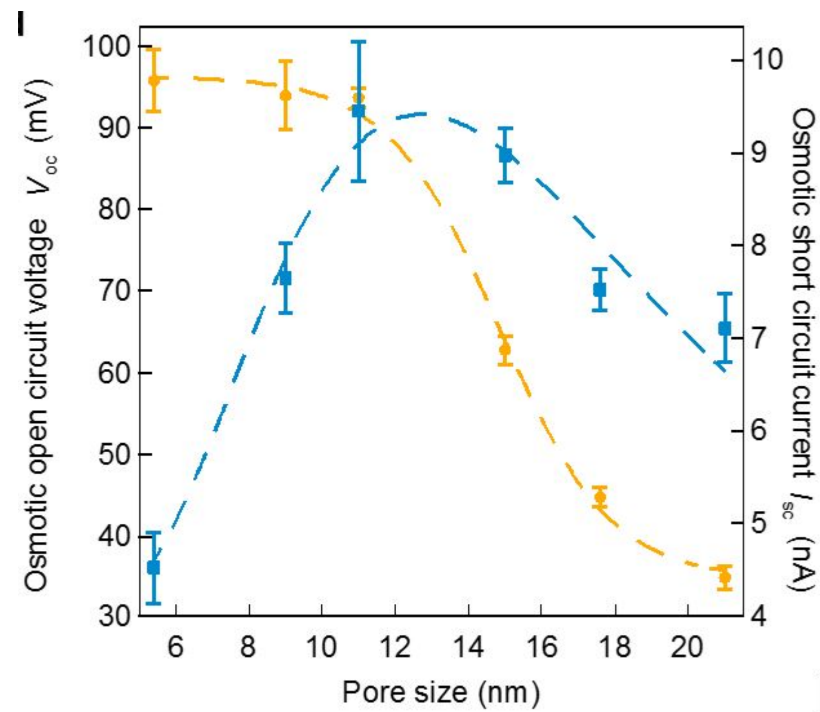




Results: Pore Size Effect

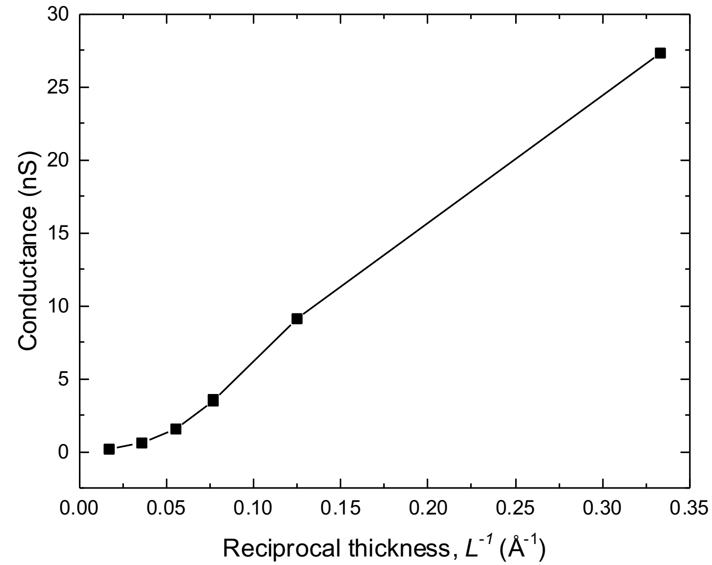
- A non-monotonic relationship between short circuit current and pore size in both the experiment and continuum analysis
- For larger pore, the selectivity of the pore decreases
- This results in mixing of ions with an equal and opposite diffusive current

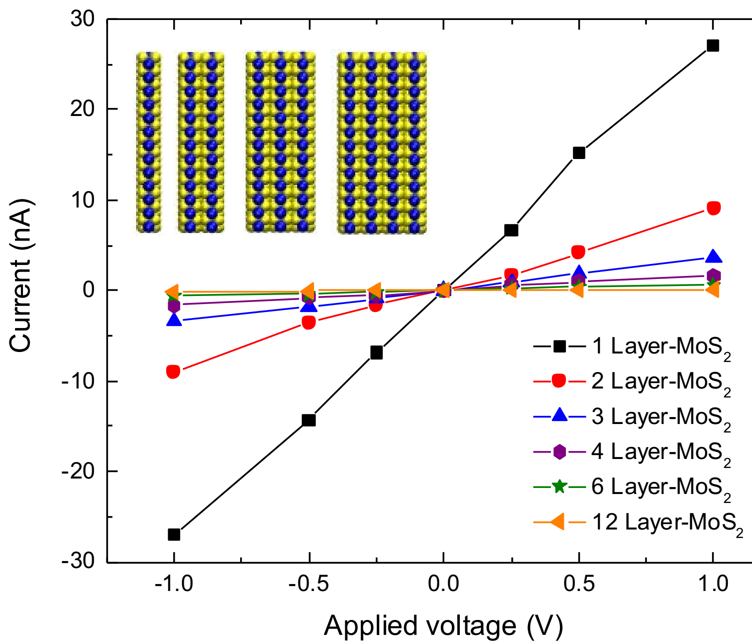


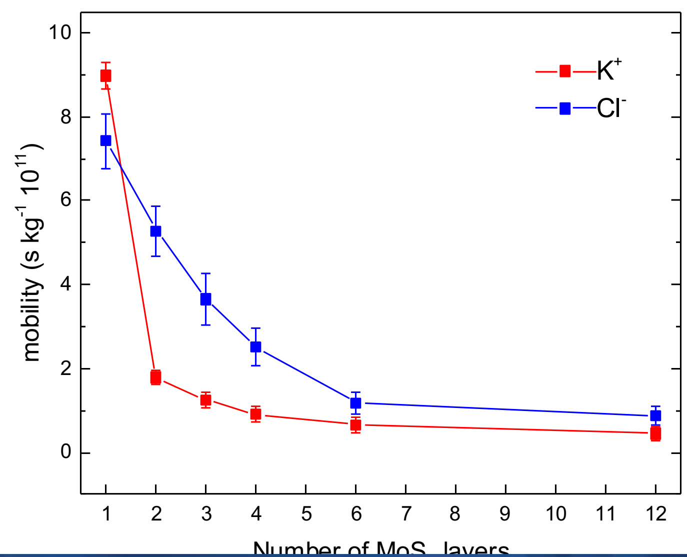


Results: Effect of Thickness

- Symmetric concentration of 1M KCl in MD
- Variation of conductance with inverse thickness is not linear
- ionic mobility also influences the conductance

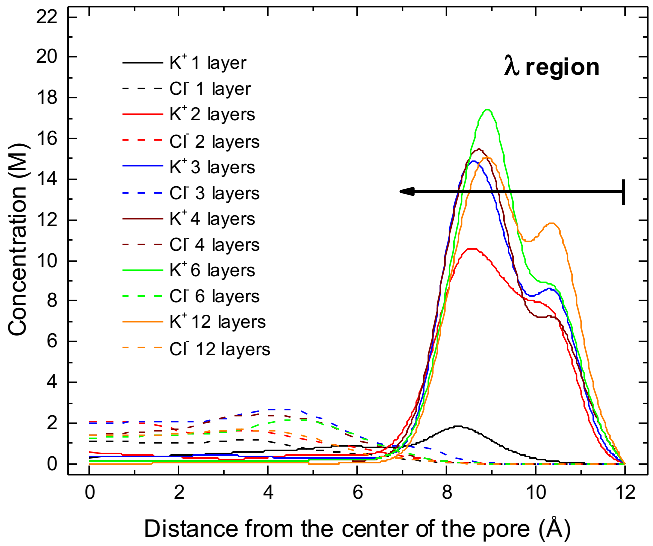




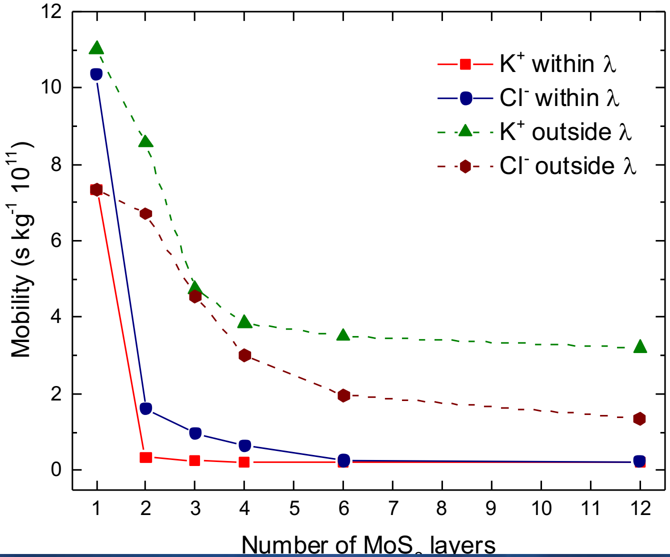


Results: Mobility & Double Layer

- Abrupt reduction is due to the strong adsorption of counter-ions to the surface
- A double layer near the surface
- Mobility of ions decreases sharply within double layer
- Residence time increases for multilayer membranes

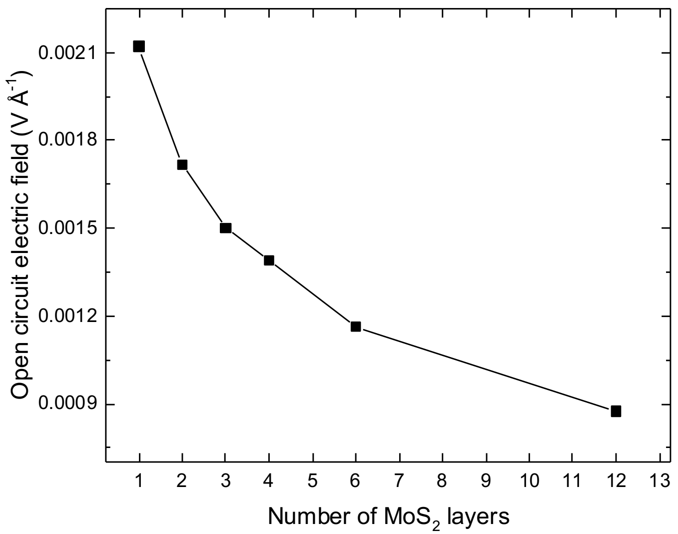


Number of MoS_2 layers	Residence time of K^+ within λ [ns]
1	0.08
2	1.52
3	3.46
4	5.53
6	7.26
12	15>



Results: Power & Thickness

* Maximum power is proportional to both the conductance and the square of open-circuit voltage
* A multilayer MoS2 reduces the power substantially
* Power for a twelve-layer MoS2 is ~3% of that of the single-layer membrane



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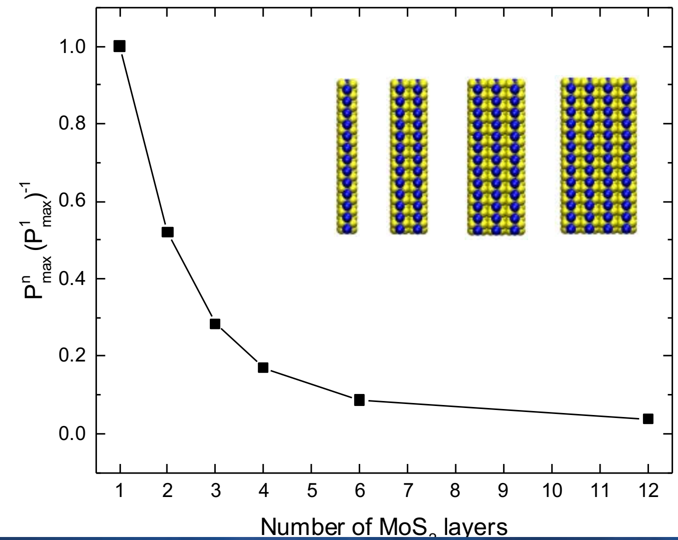
This work	10^6	0.65 nm
Multilayer MoS_2 (Simulations)	30000	7.2 nm



Conclusions & Acknowledgment

* MoS2 membranes are promising in power generation from chemical potential
* Giant power is generated, 10^6 W m^{-2}, 3 orders of magnitudes higher than previously reported results
* Thinness of a single-layer MoS2 is the key to this giant power generation
* In addition to length effect, the ion mobility decreases with length of membranes (multilayer MoS2)
* Non-monotonic short circuit current behavior is due to the competition between diffusive and migration currents
* The decrease in short circuit current with pore size originates from the loss of selectivity in large pores

Special thanks to Blue Waters for making this possible!

Thanks for your attention!

Questions?