Non-linear electrokinetic flow and ion transport near/in the nanofluidic devices: Insights using molecular dynamics simulations

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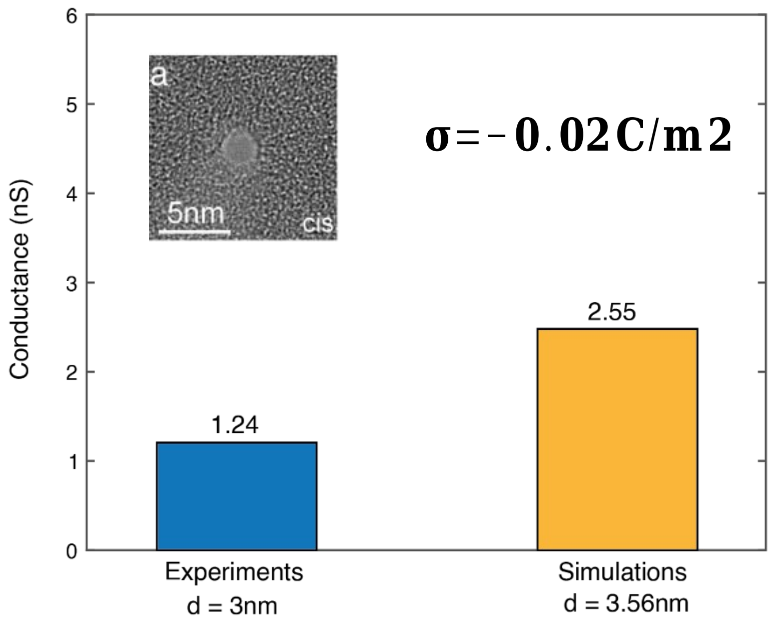
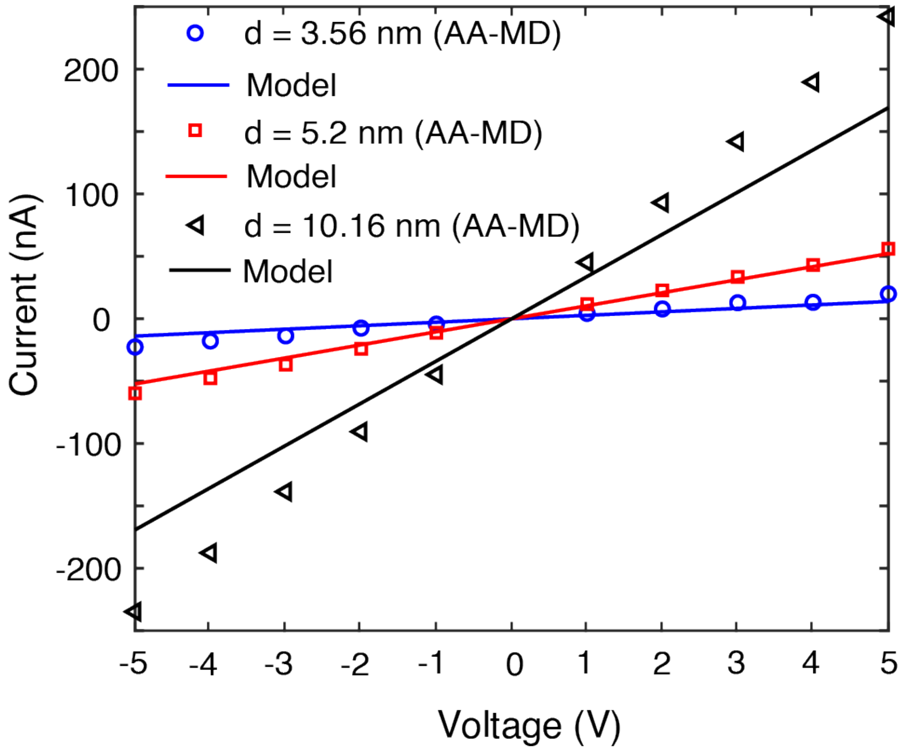
The MD data may be put in perspective with the corresponding data in physical units with reference to some realizable practical solid state nanopore device.

Nanopore Conductance



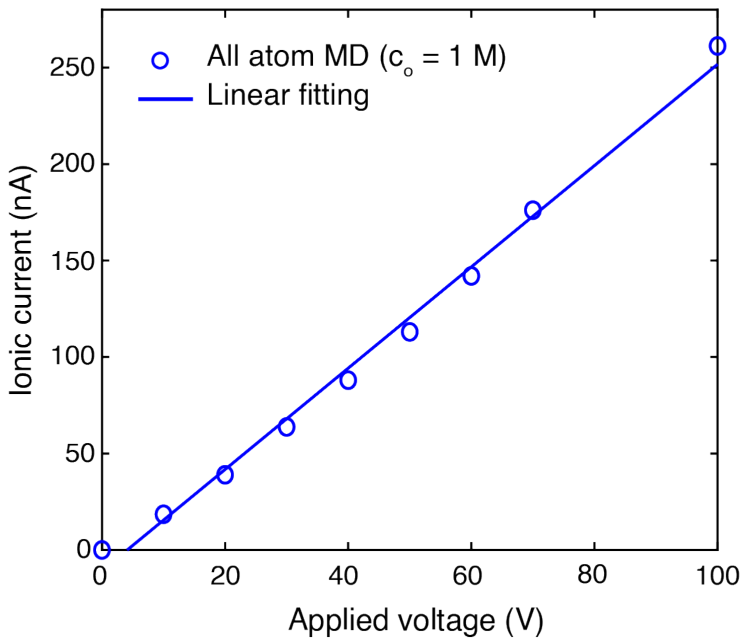


Biophys J 87, 2086–97 (2004).
PNAS 102, 10445-10450 (2005).

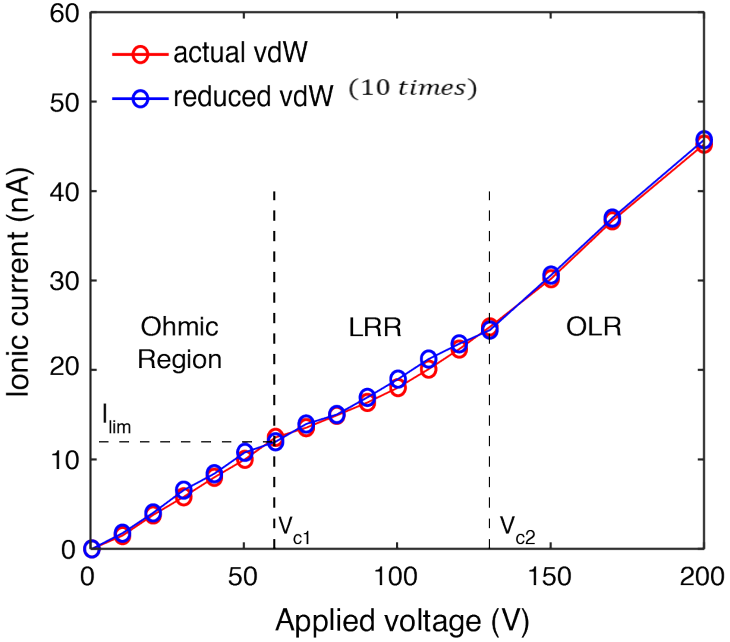
We compare the nanopore conductance from the MD simulations with the solid-state nanopore device used in the experiments. The nanopore conductance values are in the same order as the experiments and observe the linear I-V characteristics in the same voltage range. However, the conductance value is found to be higher than the experiments since the exact shape, and surface charge distribution on the pore is not known in experiments.

Sensitivity of the results with variation in the MD simulation data may be summarized to isolate the key parameters influencing the final results.

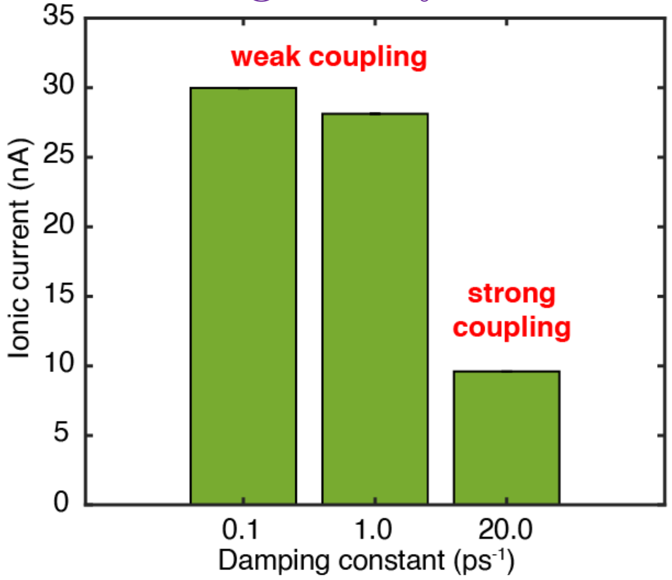
Bulk concentration



vdW parameters



Langevin dynamics



$$m_i \frac{d^2 r_i}{dt^2} = -m_i \gamma \frac{dr_i}{dt} + F_i$$

- damping constant

We summarize the MD simulation key parameters that influence the final results of I-V characteristics. The key parameters include bulk concentration, vdW parameters, thermostat dampening coefficients.

Noises inevitable in MD simulations may be compared with the noises stemming from the experimental situations, to enable isolating the noises from the signal.

MD simulations

1/f noise	Thermal noise
Dielectric noise	MD noise

Experiments

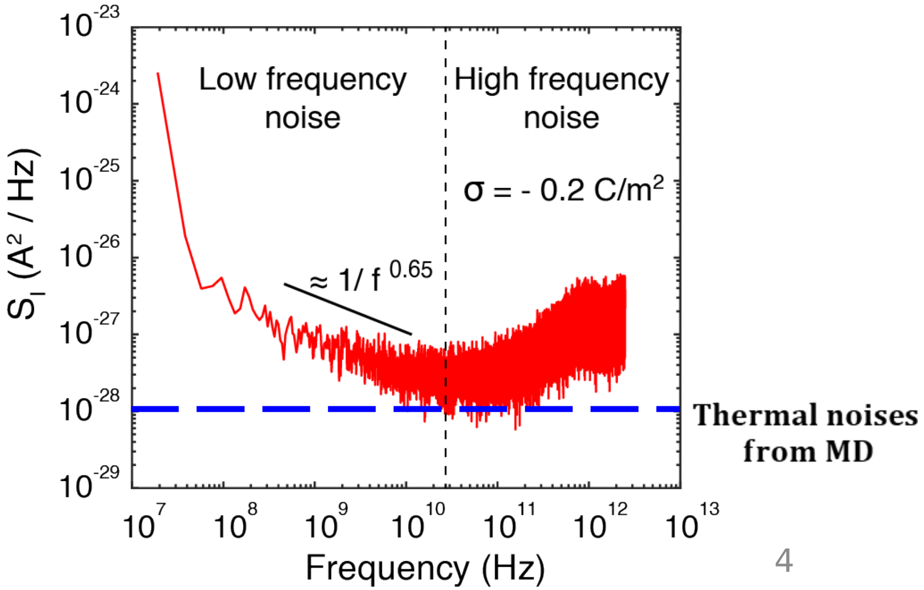
1/f noise	Thermal noise
Dielectric noise	Capacitor noise
Electrode noise	

MD noise sources

- Integrating EOM
- Constraint dynamics
- Finite size effects of atoms
- Temperature control

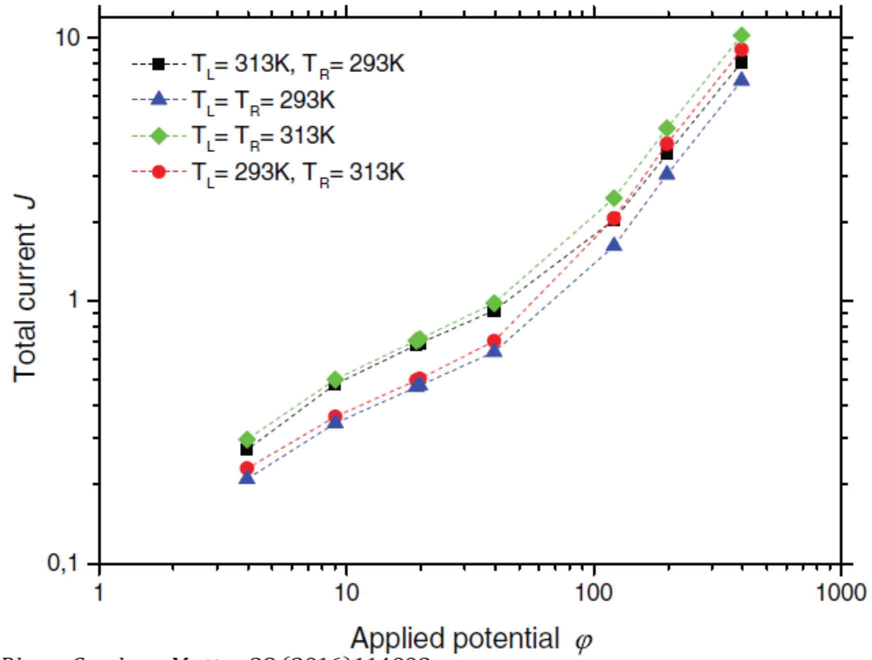
- To understand the MD generated noises, we ran the simulations without considering nanopores, i.e., only the electrolyte solution. However, the results showed that thermal noises ($S_T = O(10^{-28})$) match the theoretical formulation) dominate even in the absence of the surface charge and nanopore effects.

- As the MD generated noises are thermal noises, they cannot affect the scaling of the 1/f noises present in the nanopores.



Nonlinear electrokinetics are associated with several facets, including thermally driven nonlinear features. What are the roles of those other sources of nonlinearity in altering the final voltage-current characteristics?

Temperature effects



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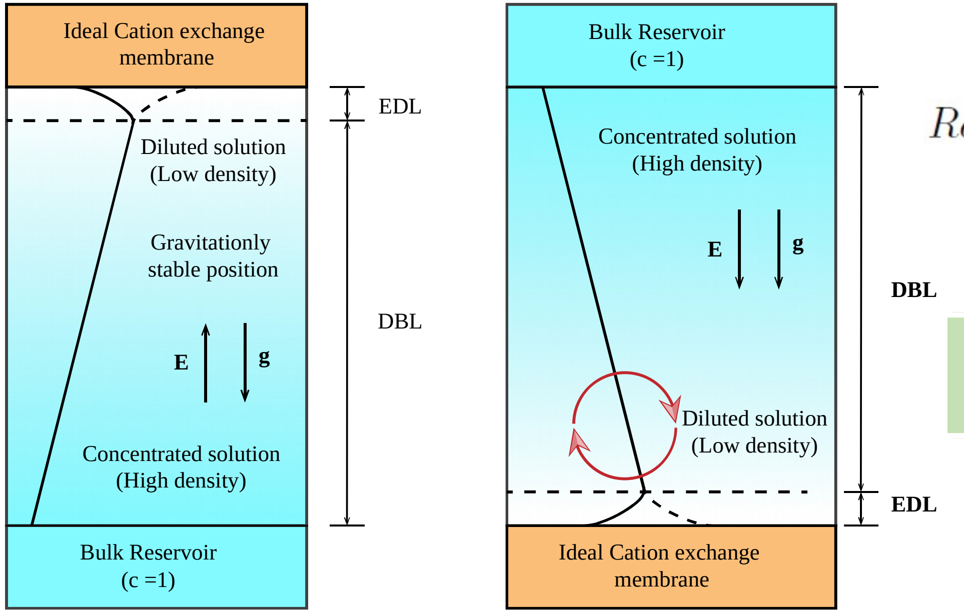
I-V characteristics are sensitive to the thermally driven effects. However, these variations are attributed to the local variation of the physical properties of the ionic liquid with temperature distribution, which affects the ion selectivity of the devices.

Gravitational effects



Stable *Unstable*

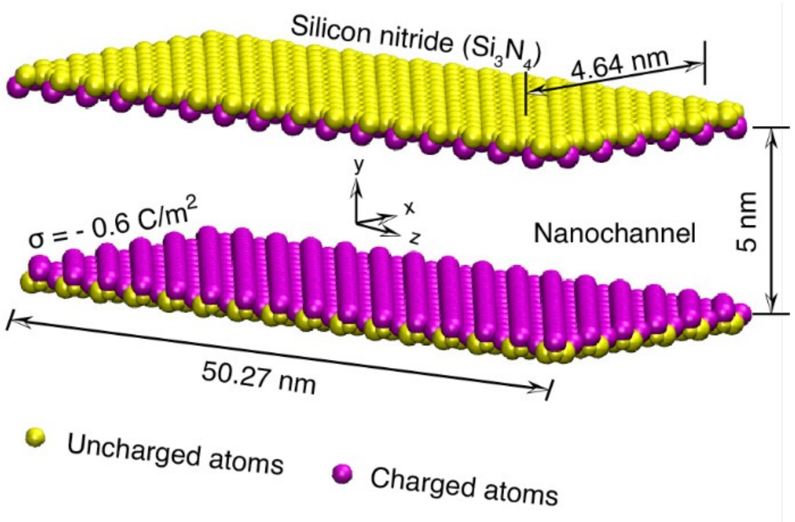
$$Ra = \frac{\Delta \rho g L^3}{\rho \mu D}$$

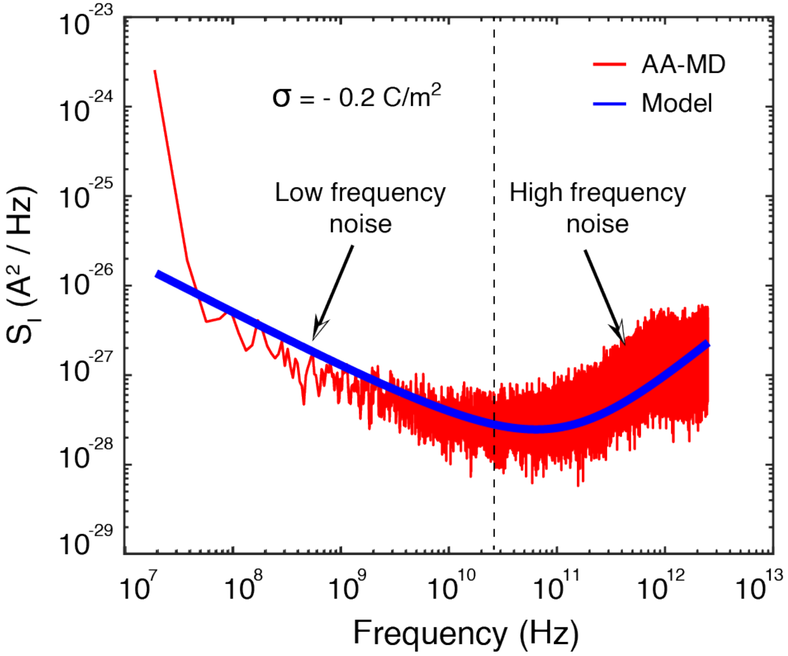
For 0.1mM, $Ra > 1000$

L >1.4 mm

The dominance of this gravitational effect depends on the position of the ion-selective device and Rayleigh number ($Ra > 1000$). For the gravitationally stable position, these effects are small, whereas, for unstable positions, these effects depend on the Rayleigh number.

What is the anticipated scalability between the MD simulations and experimentally observed features of nanoscale electro-fluidic devices?

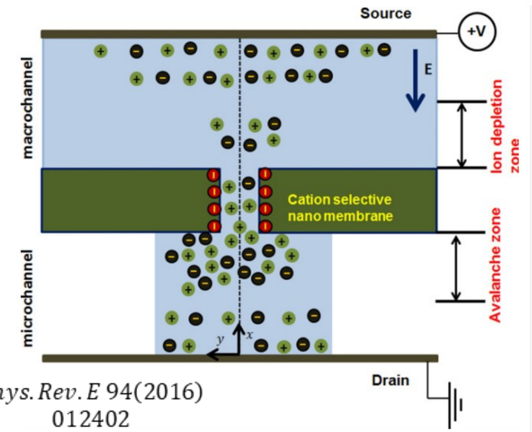




The MD simulations can be scaled up to the length scale of 100 to 150 nm (includes 6 to 10 million atoms). However, the quantitative comparison between the experiments and MD simulations cannot be made due to the limitations of MD simulations accessible to larger time and length scales. Moreover, the models/scaling laws developed using the MD simulations can be scaled to explain the experimentally observed phenomenon using nanofluidic devices.

What are the specific applications which may benefit from the outcome of this thesis? How?

Nano fluidic diodes



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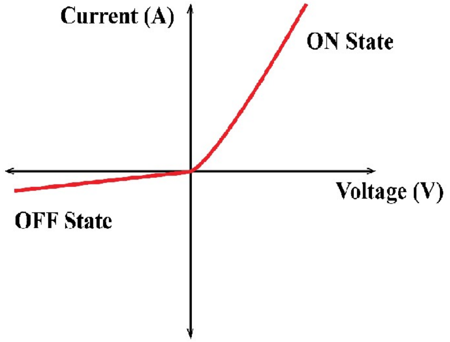
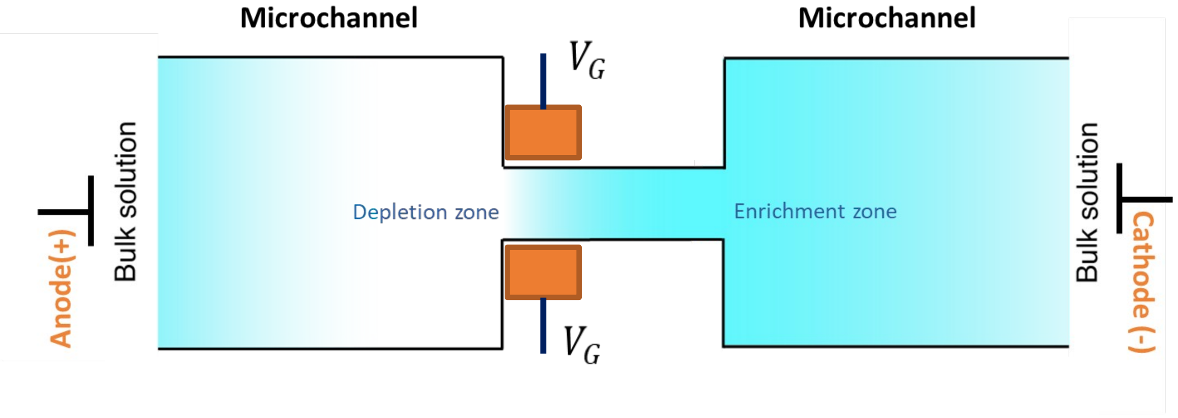
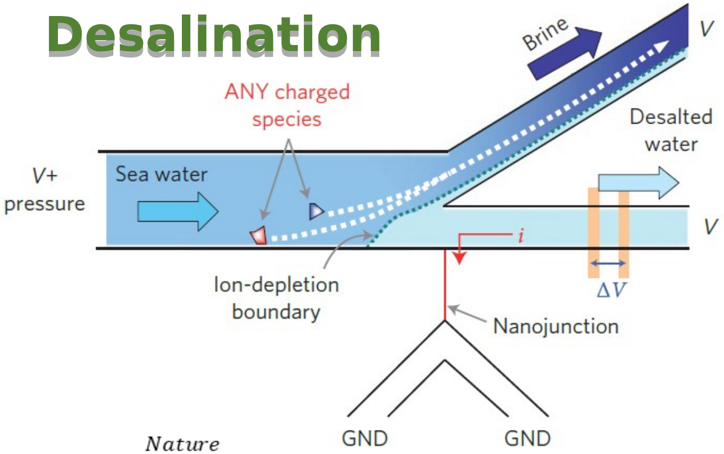


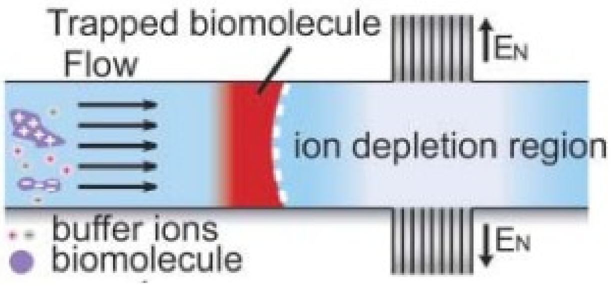


Sea Water Desalination



Nature Nanotechnology 5 (2010) 297

Biomolecule Preconcentration

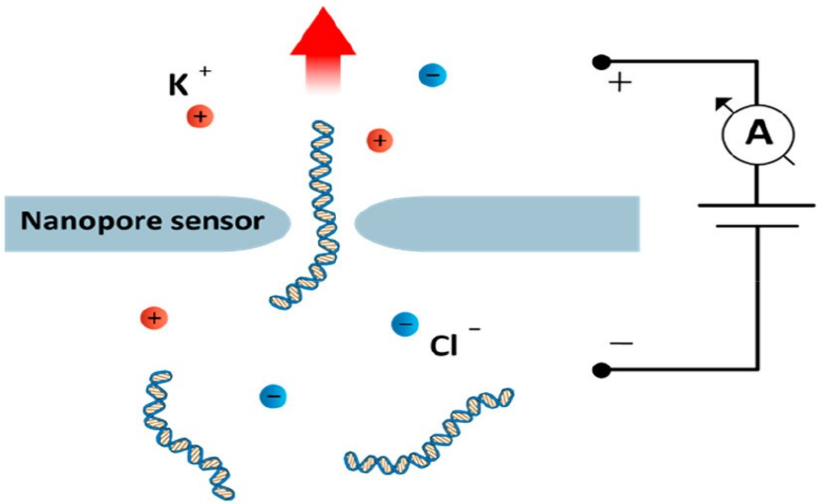


Lab Chip 8 (2008) 392–394

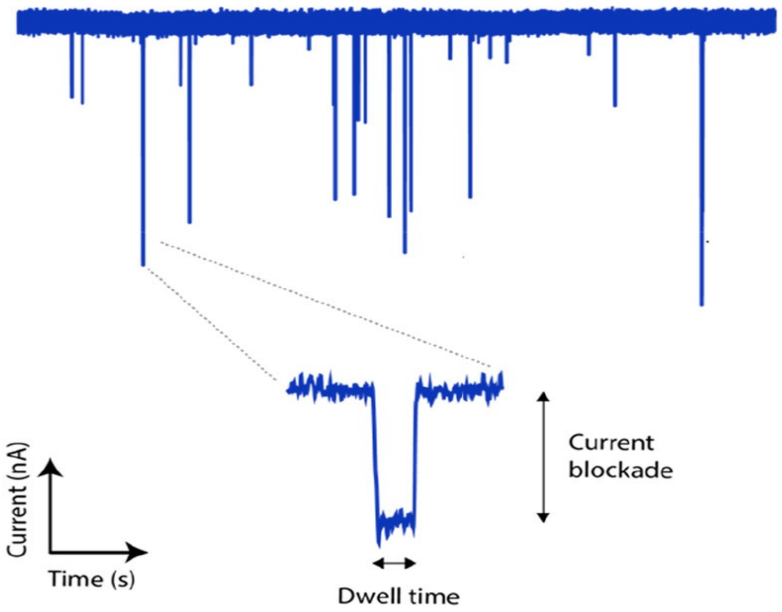
- I-V characteristics are sensitive to the concentration and potential distribution inside the devices.

- By controlling the potential distribution with the help of gate voltages (V_G), the ESC region can be tuned to improve the efficiency of these mentioned applications.

DNA sequencing and Bio – molecule sensing



ACS Nano. 1338, 14(2021)



$$S_I = S_{IL} + S_{IH}$$

$$= \frac{\alpha' I^2}{N_C f^\alpha} + \frac{4K_b T}{R_P} + 8\pi K_b C_P T D f$$

Low frequency noise + **Thermal noise** + **Dielectric noise**

By controlling the various sources of noise in the nanopore, the Signal-to-Noise (SNR) ratio can be improved, which increases the efficiency of the nanopore sensing devices.

Thank You!