Theoretical prototype of a Hodgkin-Huxley neuron with 2D nanofluidic memristors

How to build a neuron with salty water?

Paul Robin, Nikita Kavokine, Lydéric Bocquet
Micromégas, Ecole Normale Supérieure, Paris

Ref.: P. Robin, N. Kavokine, L. Bocquet, Science, in revision.

Man versus machine: a two-sided game

AlphaGo vs Lee Sedol (2016)

VS

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vs

4 – 1

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VS

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1920 CPUs, 280 GPUs $\sim$ 1 MW
10^6 bananas/day

1 brain $\sim$ 20 W
2 bananas/day

Why?

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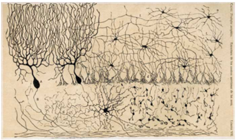
- Von Neumann architecture

- Highly parallel



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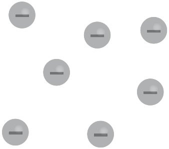

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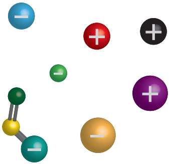
- Highly parallel
- Ions with different "flavors"



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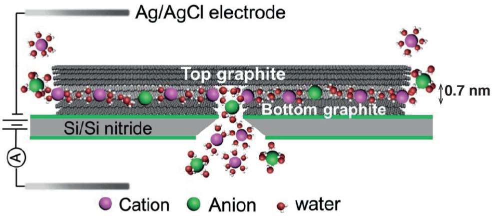
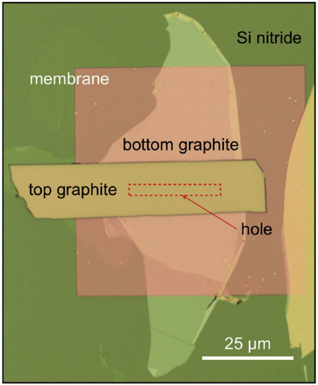
Can we build a nanofluidic computer?
(or at least building blocks)

A key nanofluidic device: the angstrometric slit

Electrolyte confined to molecular level between two sheets





Effects of molecular nature of water/ions?

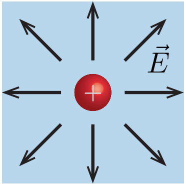
No clear theoretical framework

Radha *et al.*, Nature (2016); Esfandiar *et al.*, Science (2017); Mouterde *et al.*, Nature (2019)

How do ions behave in extreme confinement?

Confinement of interactions

Bulk water



$$V_{3D} = \frac{q}{4\pi\epsilon_0\epsilon_r r}$$

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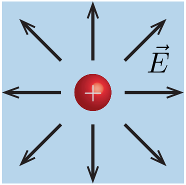
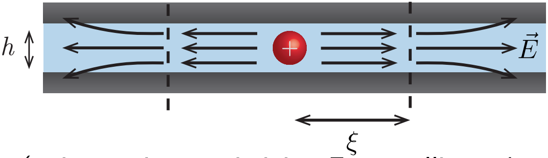


'2D$^+$' confined water, $\xi \sim 14\,\text{nm}$



(anisotropic permittivity, Fumagalli *et al.*, Science 2018)

$$V_{3D} = \frac{q}{4\pi\epsilon_0\epsilon_r r}$$

$$V_{2D^+} = -\frac{q}{4\pi\epsilon_0\epsilon_r \xi} \log \frac{r}{r+\xi}$$

Confinement of interactions

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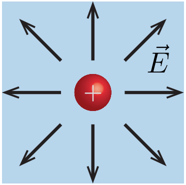

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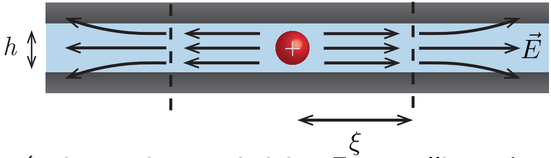

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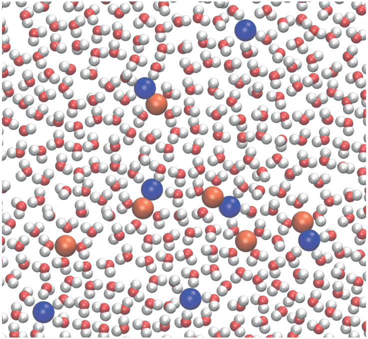
Confinement also impacts interactions

Reinforced interactions in confinement: Bjerrum pairs



MD simulation of NaCl in 2D monolayer water

Bjerrum pairs

Normally only observed in **weak electrolytes**

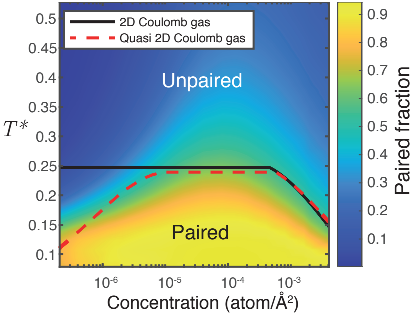
First predicted in 1D confinement (Kavokine *et al.*, Nature Nano., 2019)

Confinement makes water a poor solvent

Reinforced interactions in confinement: Bjerrum pairs

Strengh of interactions parameter:

$$T^* \sim k_B T \frac{4\pi\epsilon\epsilon_r\xi}{q^2}$$



Numerical/Analytical phase diagram

Kosterlitz–Thouless transition

Bjerrum pairs

Normally only observed in **weak electrolytes**

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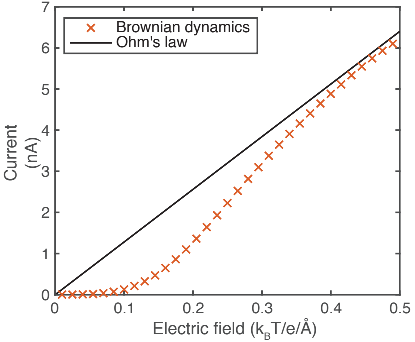
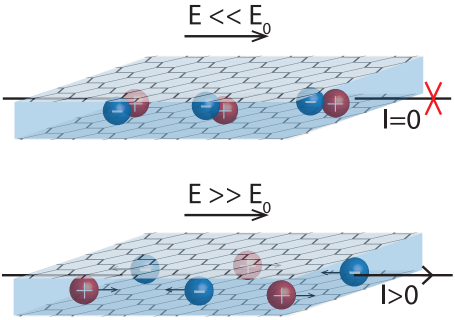
Confinement makes water a poor solvent

Wien effect (Onsager, 1934):

Pairs are neutral, do not conduct, but break under a strong voltage

Voltage-gated ion channels





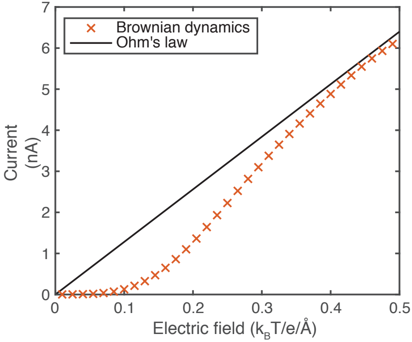
Artificial ion channels

Why are pairs interesting?

Wien effect (Onsager, 1934):

Pairs are neutral, do not conduct, but break under a strong voltage

Voltage-gated ion channels



2D Wien effect:

A fraction n_f of ions is "free":

$$\dot{n}_f = \frac{1-n_f}{\tau_d(E)} - \frac{n_f^2}{\tau_a} = 0$$

$$I \propto n_f E$$

$$\tau_d \propto E^{1/T^*}$$

(self-similarity argument)

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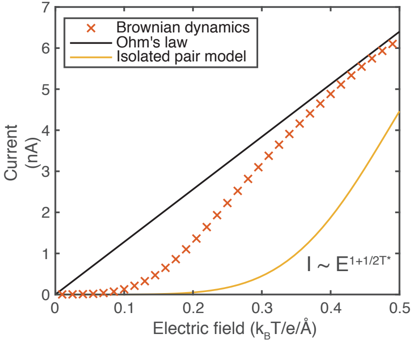

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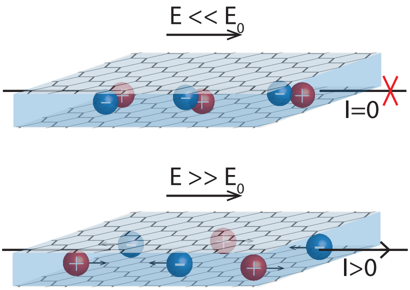
Onsager's Wien effect fails!

The problem with Wien effect: Bjerrum polyelectrolytes

Onsager's picture:



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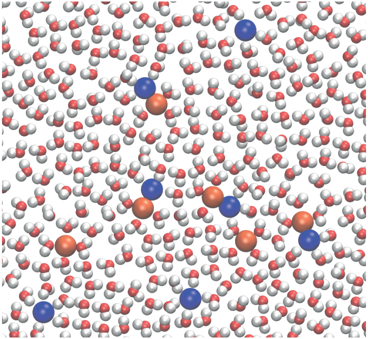

NaCl, $E = 0$

The problem with Wien effect: Bjerrum polyelectrolytes

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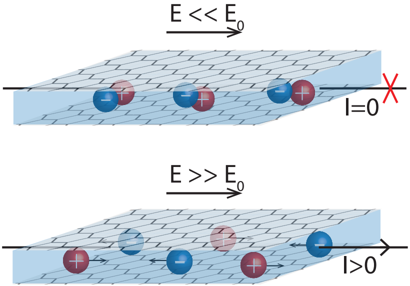

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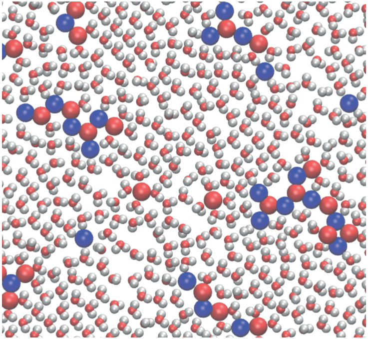
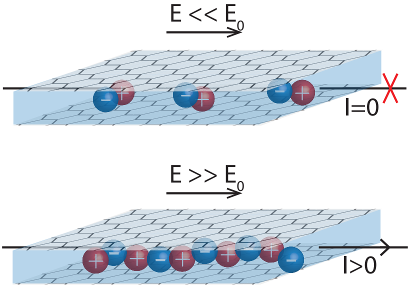
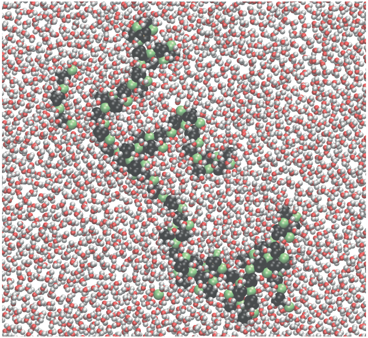


NaCl, $E > 0$

The problem with Wien effect: Bjerrum polyelectrolytes

Polyelectrolytic Wien (PEW) effect:





$CaSO_4$, $E > 0$

The problem with Wien effect: Bjerrum polyelectrolytes

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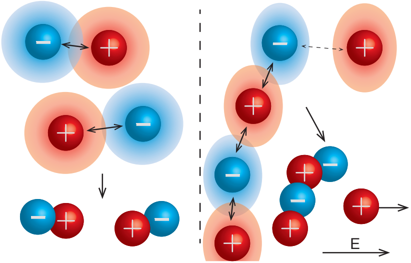
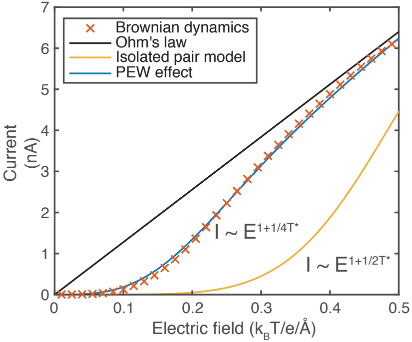


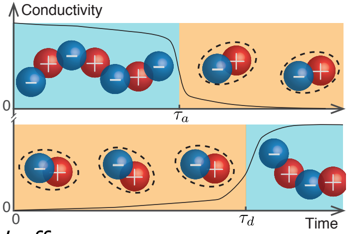
$$\dot{n}_f = \frac{1 - n_f}{\tau_d(E)} - \frac{n_f^2}{\tau_a} = 0$$

$$\tau_d \propto E^{1/2T^*}$$



MD simulations vs theory
(no fitting parameter)

Conduction memory: memristor effect



PEW effect:

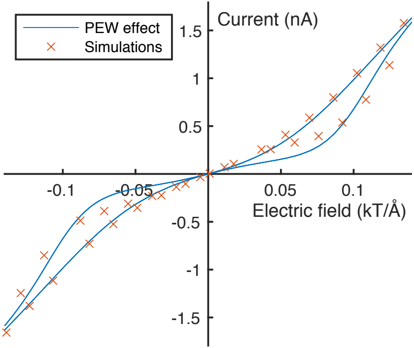
$$I \propto n_f E$$

$$\dot{n}_f = \frac{1 - n_f}{\tau_a(E)} - \frac{1}{\tau_d} n_f^2$$

n_f: % of ions in polyelectrolytes

Memristor

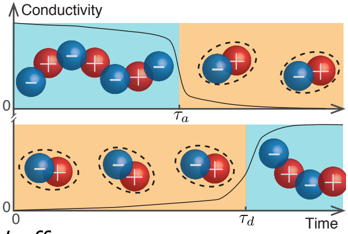
$$E = E_0 \cos 2\pi f t$$



MD simulations vs theory

Pinched ⇒ memristor

Conduction memory: memristor effect



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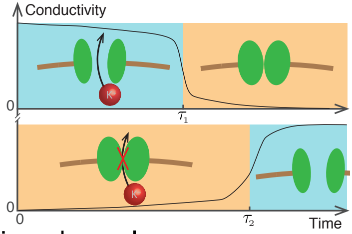


K^+ ion channel:

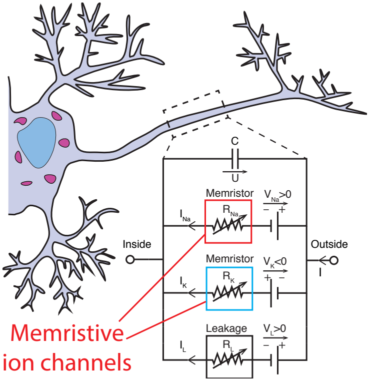
$$I = g n^4 \Delta V$$

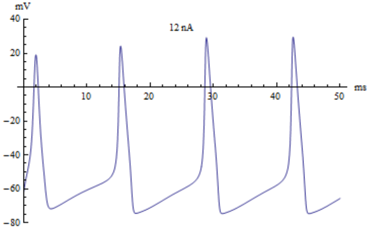
$$\dot{n} = \frac{1 - n}{\tau_1(\Delta V)} - \frac{n}{\tau_2(\Delta V)}$$

n: 'activity' of the channel
(Hogdkin and Huxley, 1952)

also a memristor!

Hodgkin-Huxley neuron model



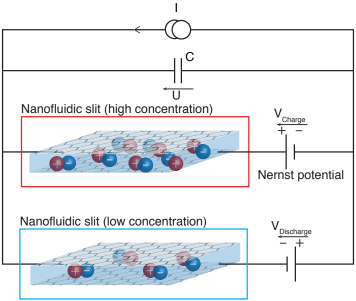


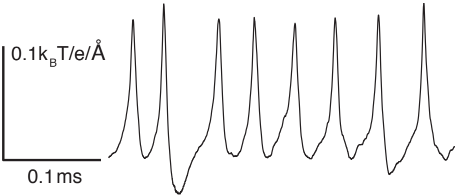
Hodgkin-Huxley model (Nobel 1963)

Action potential train (Wikipedia)

Prototype nanofluidic neuron

Fully simulated with molecular dynamics:

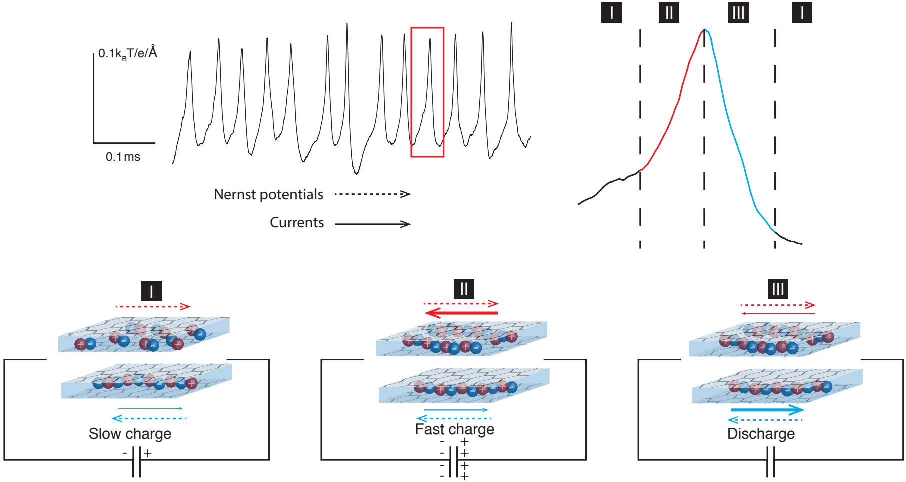




Nanofluidic neuron
(Two coupled simulation boxes)

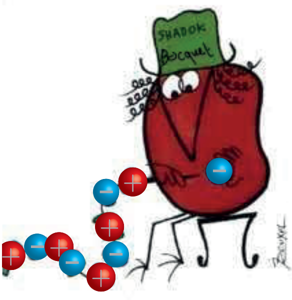
Action potential train

Spiking mechanism



Conclusion

- Ion clusters under confinement



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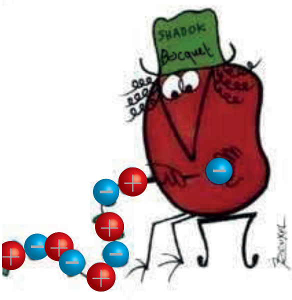

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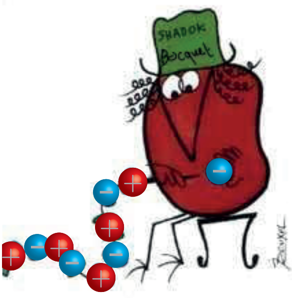

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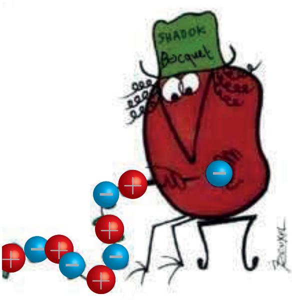

Take-home message

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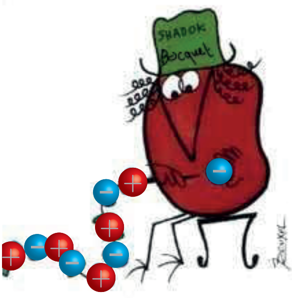

Take-home message

- Confinement also impacts interactions

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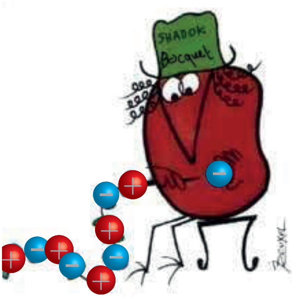

Take-home message

- Confinement also impacts interactions
- Large structures ⇔ Long correlation times ⇔ Memory

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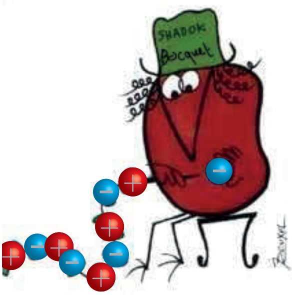

Take-home message

- Confinement also impacts interactions
- Large structures ⇔ Long correlation times ⇔ Memory
- **Experimentally accessible!**

...Dynamical nanofluidics is worth the journey!

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