Scaling for rectification of bipolar nanopores

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Nanopores are nanoscale channels embedded in a membrane providing a controlled transport of ions between the two bulk phases on the two sides of the membrane. The nanopore's radius, R, is in the nanometer range, comparable to the Debye length, λ_D.

Charge patterns are chemically deposited on the inner wall of the engineered nanopore providing different output signals for different input parameters. From the relation of the input and output signals a device function can be generated. In the case of a bipolar nanopore (the wall of the pore is negatively charged in one half and positively charged in the other half of the pore along the pore axis), the device function is ionic current rectification defined as ICR = $(I^{ON} - I^{OFF})/(I^{ON} + I^{OFF})$, where I^{ON} and I^{OFF} are total currents at the forward and reversed bias signs of the voltage, respectively. The scaling of the rectification of the nanopore means that rectification is a unique, smooth and monotonic function of a well defined scaling parameter.

We showed that the modified Dukhin number introduced in Ref. [1] for selective nanopores and defined as

$$mDu = 8 l_B \lambda_D |\sigma| H U / (e R U_0)$$

is a suitable scaling parameter for the bipolar nanopore, where H is the length of the pore σ is the surface charge density, and l_B is the Bjerrum length, U is the voltage, and U_0 is a reference voltage.

We use simple models based on the primitive model of electrolytes and study those models with the Nernst-Planck (NP) transport equation coupled either to the Local Equilibrium Monte Carlo method (NP+LEMC) [2] or the Poisson-Boltzmann theory.

The latter, known as the Poisson-Nernst-Planck (PNP) theory, is a mean-field theory. We show that scaling is fundamentally a mean-field phenomenon. We showed that the NP+LEMC and PNP results agree for 1:1 electrolytes where ionic correlations are weak [3,4], while deviations are found from the mean-field scaling behavior for 2:1 and 3:1 electrolytes at large surface charge densities [5]. Thus, scaling can be considered as a measure of the applicability of mean-field theories.

REFERENCES

[1] Zs. Sarkadi, D. Fertig, Z. Ható, M. Valiskó, D. Boda, *J. Chem. Phys.,* 2021, **154**(15):154704.
[2] D. Boda and D. Gillespie, *J. Chem. Theory Comp.,* 2012, **10**(8):824-829.
[3] D. Fertig, Zs. Sarkadi, M. Valiskó, D. Boda, *Mol. Sim.,* 2021, in press
[4] D. Fertig, B. Matejczyk, M. Valiskó, D. Gillespie, D. Boda, *J. Phys. Chem. C.*, 2019, **123**(47):28985-28996.
[5] D. Fertig, M. Valiskó, D. Boda. *Phys. Chem. Chem. Phys.,* 2020, **22**(34):19033-19045.

FIGURES

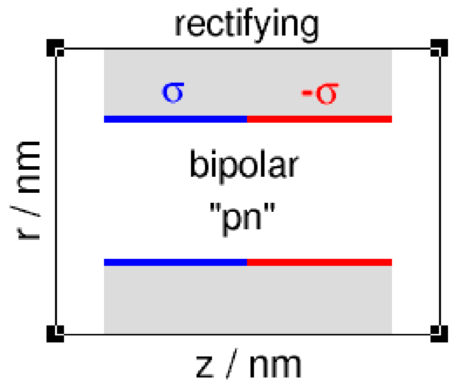

Figure 1: The bipolar nanopore's surface charge pattern is asymmetric, its device function, therefore, is rectification.