Theoretical insights of electrolyte transport in nanopores

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Fundamental understanding of ionic transport at the nanoscale is essential for developing biosensors based on nanopore technology and new generation high-performance nanofiltration membranes for separation and purification applications.

After a general introduction on the theoretical modeling of ionic transport in nanopores, we present a mesoscopic theoretical approach for the electrolyte conductivity inside nanopores. The model considers explicitly ion advection by electro-osmotic flow, possible flow slip at the pore surface (when the pore is hydrophobic) [1], dielectric exclusion of the ions [2], hard core repulsion between ions [3], and surface charge regulation [4]. Various regimes where the conductivity has a relatively simple analytical expression are identified.

The theory is then compared to experimental measurements of ionic transport through single putatively neutral hydrophobic nanopores and with a well controlled cylindrical geometry [1] and through single wall carbon nanotubes [5]. We focus on the dependence of the nanopore conductance with the reservoir ionic concentration, showing various behaviours depending on the experimental conditions.

- S. Balme, F. Picaud, M. Manghi, J. Palmeri, M. Bechelany, S. Cabello-Aguilar, A. Abou-Chaaya, P. Miele, E. Balanzat, J.-M. Janot, Ionic transport through sub-10 nm diameter hydrophobic nanopores : experiment, theory and simulation, Scientific Reports 5, (2015) 10135
- [2] S. Buyukdagli, M. Manghi, J. Palmeri, Ionic capillary evaporation in weakly charged nanopores, Phys. Rev. Lett. **105**, 158103 (2010)
- [3] B. Loubet, M. Manghi, J. Palmeri, A variational approach to the liquid-vapor phase transition for hardcore ions in the bulk and in nanopores, J. Chem. Phys. 145, (2016) 044107
- [4] M. Manghi, J. Palmeri, K. Yazda, F. Henn, V. Jourdain, Role of charge regulation and flow slip on the ionic conductance of nanopores : an analytical approach, arXiv:1712.01055 (2017)
- [5] K. Yazda, S. Tahir, T. Michel, B. Loubet, M. Manghi, J. Bentin, F. Picaud, J. Palmeri, F. Henn, V. Jourdain, Voltage-activated transport of ions through single-walled carbon nanotubes, Nanoscale, 9, (2017) 11976