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Ionic transport through metallic and semiconducting carbon nanotubes

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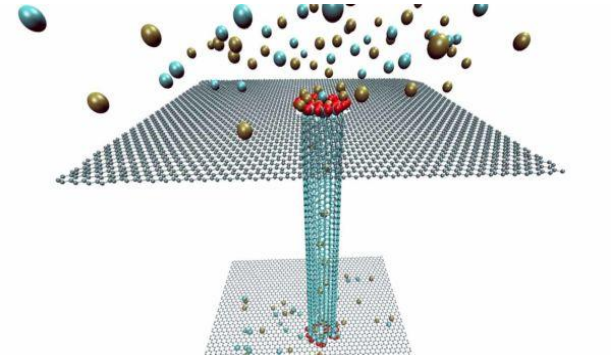
Abstract

Single-Walled Carbon Nanotubes (SWCNTs) are amongst the most promising materials for an advanced generation of electro-ionic media, thanks to their small diameter (0.7 to 2nm) offering the optimal electrostatic coupling between the channel wall and the translocating ions, together with minimal coupling with electrolyte reservoirs. Besides, the very low friction on the nanotube wall allows a fast transport of electrolytes. Moreover, SWCNTs can be either conductor of electrons (metallic) allowing to control their surface charge and thereby the transport of ions through their inner channel ; or semiconducting which are promising electronic sensors.(1)

Our work aims to explore several phenomena through a theoretical point-of-view. The first insight seeks to compare, with an analytical approach, three physical mechanisms at the origin of ion exclusion in nanopores : the dielectric exclusion, the Born solvation self-energy, and the solvation energy related to Debye-Hückel parameters. (2)

The second insight looks at the impact of SWCNTs chirality on the surface charge provoked by the application of a gate voltage through a metallic electrode. In order to do so, we have to look on how the nanopore capacitance is governed by his electronic density of states. We will thus question ourselves about how it is important to take quantum capacitance into account in an ionic transport model through a SWCNTs. (3)



(1) Balme, S., Picaud, F., Manghi, M. et al. Ionic transport through sub-10 nm diameter hydrophobic high-aspect ratio nanopores: experiment, theory and simulation. Sci Rep ***5,*** *10135 (2015). https://doi.org/10.1038/srep10135*

(2) Hennequin,T., Manghi, M., Palmeri, J., Competition between Born solvation, dielectric exclusion, and Coulomb attraction in spherical nanopores, T.Hennequin, M.Manghi, J.Palmeri, arXiv:2104.14824v1 (2021)

(3) Hennequin,T., Manghi, M., Palmeri, J., Influence of the quantum capacitance on the transport of electrolytes through CNTs, (coming soon)