Minicolloque n° MMB15 **X Oral** **□ Poster**

CONFINED MEDIA: FUNDAMENTAL TO APPLICATION

Theoretical investigations on ionic conductance at nanoscale: pore geometric parameters effect.

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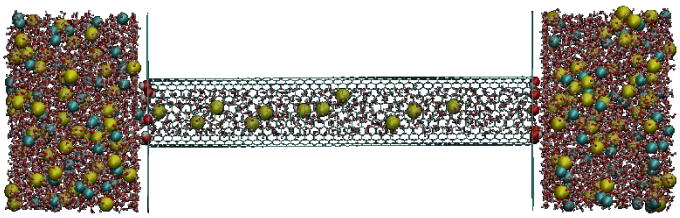
Ultra-efficient transport of water and ions at nanoscale is expensively studied for graphene nanopores during the past decades. Many experimental fabrication strategies and devices are developed for the manufacture of controllable porous membranes with various applications in nanotechnology area: filtration1, water desalination2, imaging living cells3...

Theoretical investigations are also of great interest to provide supplementary information to experimental studies. Herein carbon nanotubes are used to mimic biological protein channels in cell membranes due to their smooth inner structure and the compromise of a very simple composition for tremendous variety of properties. A flow of solvated ions moving inside the carbon nanotube under the application of an external potential difference allowed relevant measurements of the ionic current established in the internal area of the tube. Our theoretical studies based on molecular dynamics simulations aims at detecting the effect of the geometric parameters of the pore (length, chirality, diameter and chemical functions at the ends) on the conductance of the system. We will in particular show that the conductance of the carbon nanotube can importantly vary depending on the experimental preparation of the nanotube.



Ion transport inside (13,13) edge-functionalized carbon nanotube connecting two reservoirs of electrolytes.

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