Biological channel mimics for use as desalination membranes

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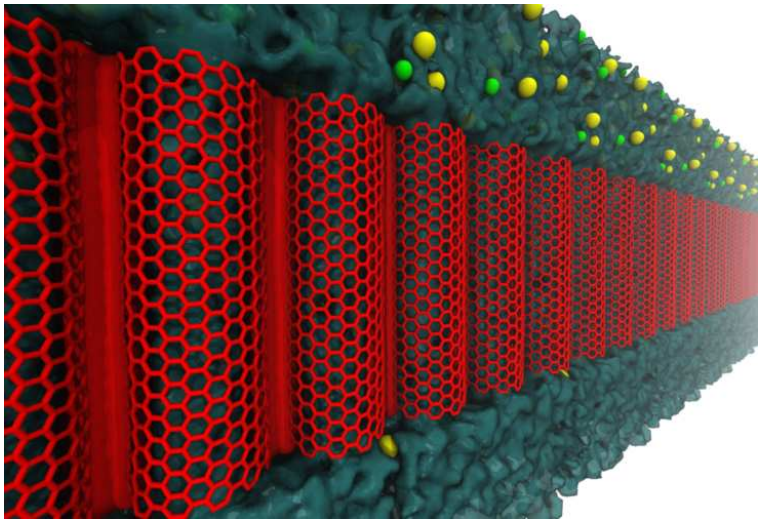
Biological channels display a wide and varied range of properties, including the degree of water permeation and the ability to filter unwanted species. We have used these channels as inspiration for developing our own synthetic channels for specific purposes: desalination and water purification. We have conducted long time scale molecular dynamics simulations on carbon nanotube based membranes (see Figure) to elucidate various properties of these hydrophobic pores. The dependence of pore width, length and functionalisation, as well as the effect of salt (NaCl) concentration and pressure, on water permeability and salt rejection has been determined. We find that:

1. wider pores have a greater permeability, but lower salt rejection,
2. permeability is dependent on pore length (*i.e.* water flow through these hydrophobic pores is not frictionless),
3. functionalisation alters salt rejection and reduces permeability,
4. increasing salt concentration generally increases salt rejection, but lowers permeability,
5. there is a linear response of permeability with pressure, but a non-linear response of salt rejection with pressure.



An array of carbon nanotubes (red) forming a membrane that is highly permeable to water (blue surface), but not sodium (yellow) and chloride (green) ions.