Mimicking biological ion channels using nanotubes

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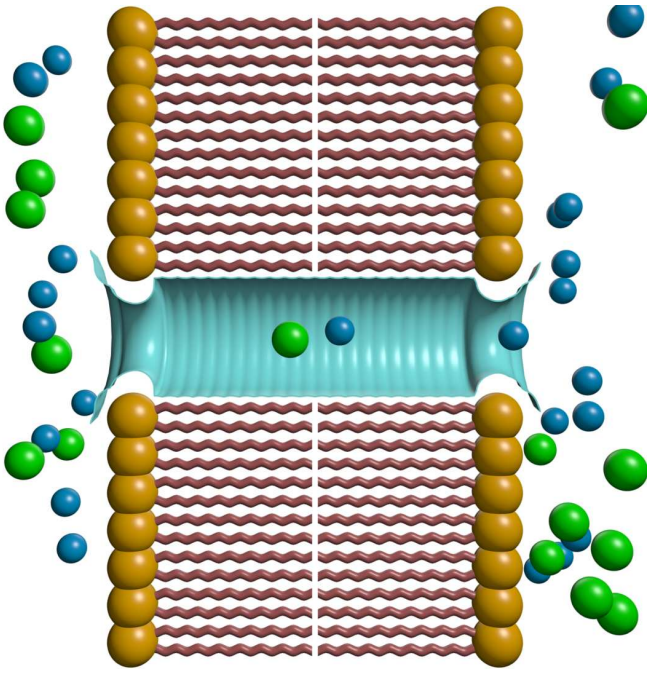
Biological ion channels are selectively permeable to specific ionic species, and regulate the flow of ions across the cell membrane. They maintain the resting membrane potential, generate propagated action potentials in nerves and control a wide variety of cell functions. We report that hollow nanotubes constructed from carbon atoms, and with hydrogen, carbonyl or carboxylic acid terminated ends, have the ability to mirror some of the important functions of various biological ion channels. In particular, these carbon nanotubes (CNTs), embedded in a lipid bilayer (illustrated in Figure), are selectively permeable to cations or anions, depending on their terminated ends and diameter. They broadly mimic some of the permeation characteristics of the antibiotic gramicidin, chloride channels, and the mutant glycine receptor.



Using a combination of molecular and stochastic dynamics simulations (see Gordon *et al.*, 2009 for details), we characterize certain properties of these engineered nanotubes, such as the free energy profiles encountered by charged particles, the current-voltage-concentration profiles and the overall conduction mechanism. We demonstrate that CNTs can be designed such that they are selective to either cations or anions by modifying their surface chemistry. In particular, we discuss three CNTs with a length of approximately 36 Å and varying surface chemistry, namely (i) with a radius of 4.53 Å and terminated with carbonyl groups (see Hilder *et al.*, 2010 for details); (ii) with a radius of 4.53 Å and terminated with hydrogen and with two regions near the entrance and exit of the nanotube exohydrogenated (outside surface hydrogenation); and (iii) with a radius of 5.08 Å and terminated with carboxylic acid. These CNTs are shown to broadly mimic the permeation characteristics of (i) the ClC-1 chloride channel and $GABA_A$ but with conduction rates 4 times and 2 times larger, respectively (see Hilder *et al.*, 2010 for details); (ii) the antibiotic gramicidin but with a potassium current 6 times larger; and (iii) the mutant glycine receptor in which anions chaperone sodium across the channel (illustrated in Figure) but with a sodium conductance 7 times larger. These synthetic nanotubes may lead to a host of pharmaceutical products to assist in treatments such as antibacterial, cancer and cystic fibrosis in addition to potential applications as sensitive biosensors.

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