

Proton-conductive materials: Inspiration from Nature
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Gramicidin A (Figure 1, left) is a protein channel forming a narrow cylindrical pore which accommodates a single-file chain of water molecules, depicted as red spheres.

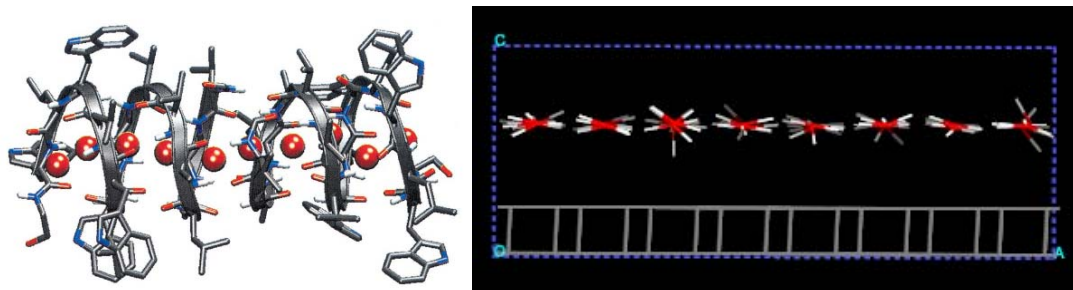


Figure 1. Left: Single-file water in Gramicidine A channel. Right: Water transport in a narrow (5 Å) graphite channel.

In addition to water, this channel is also able to conduct protons at a much faster rate than in polymer electrolyte membranes currently used in power source devices. However, the water diffusion in such confined environments (Figure 1) is much reduced; thus water is almost frozen. In this project, we seek to understand the structure and dynamics of water flowing in nanochannels made of different environments. We will use molecular simulations to analyze water transport through flexible vs. rigid channels. We will examine several possible materials and geometries in order to determine the effect of the walls on the water transport.