Design and Computational Study of an All-Carbon Water Desalination Membrane

Kyrylchuk A.,[1] Tománek D.[2]

[1]*Institute of Organic Chemistry, NAS of Ukraine, Murmanska Street 5, 02660 Kyiv, Ukraine, kyrylchuk@ioch.kiev.ua*
[2] *Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824-2320, USA, tomanek@msu.edu*

We present a previously unexplored design of an all-carbon membrane for reverse osmosis—based water desalination and employ computer modeling to gain insight into the structure of the membrane needed to achieve the best permeability and selectivity.

The proposed membrane represents a layered structure containing aligned graphite oxide flakes in its core, sandwiched in-between layers of buckypaper and carbon fibers. This assembly provides thermal stability, resilience to harsh chemicals and mechanical impact, thus responding to multiple challenges that cannot be solved using conventional polymer membranes.

Using *ab initio* DFT calculations we have modeled the permeation of water molecules and hydrated ions through layered graphite oxide. 7 Å-wide edge pores provide the best salt rejection, while marinating good water permeability. Termination of the graphene oxide edges with hydrogen atoms allows for the best permeation ratio between hydrated ions and water molecules. The hydrophilic surface of graphene oxide slows down the movement of ions along the layers, thus providing for additional salt rejection. We corroborate the possibility of concerted passage through in-layer pores, a mechanism that is accessible to water molecules but not hydrated ions.

The results of our modeling show that the optimized structure of the all-carbon membrane may turn out to be the next step in the design of advanced reverse osmosis membranes.