Progress in water desalination: Insight from *ab initio* studies

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Whereas water itself is bountiful on Earth, much of it requires treatment to make it suitable for human consumption. Lack of potable water is currently the leading cause of death, ahead of any disease. Recent progress in fabricating nanostructured carbon allotropes may bring a long-awaited paradigm shift in designing membranes that would make efficient desalination of salt water using reverse osmosis and filtration of contaminated water possible. A previously unexplored membrane design [1] based on a unique layered assembly of carbon nanostructures including graphite oxide (GO), buckypaper consisting of carbon nanotubes, and a strong carbon fabric should provide high mechanical strength and thermal stability, resilience to harsh chemical cleaning agents and electrical conductivity, thus addressing major shortcomings of commercial reverse osmosis membranes. Microscopic insight into the critical permeation of water molecules in-between GO layers and across in-layer vacancy defects in graphitic carbon can be obtained using ab initio density functional theory calculations. Results of these computational studies elucidate the reason for selective rejection of solvated Na^+ ions in an optimized layered all-carbon membrane.
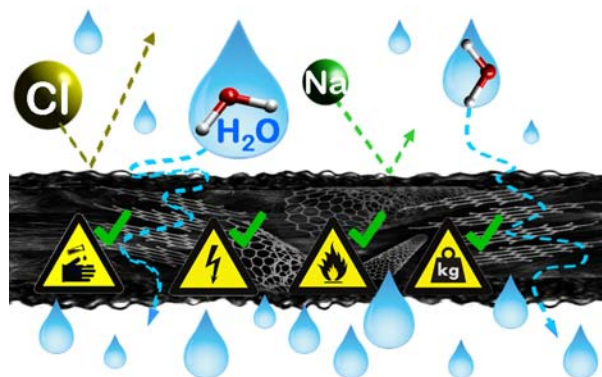

Figure 1: Design and advantages of an all-carbon membrane for water desalination and filtration.

References

[1] David Tománek and Andrii Kyrylchuk, Designing an All-Carbon Membrane for Water Desalination, Phys. Rev. Applied **12**, 024054 (2019).