Transport Diffusivity in Nanoporous Graphene

Jordan Muscatello [C, S] and Erich Müller
Department of Chemical Engineering, Imperial College London, London, United Kingdom
jlm105@ic.ac.uk

With the advent of large-scale fabrication of nanostructured carbon such as graphene and carbon nanotubes has come increased interest in the potential of these structures for use as membrane materials. Recent reports suggest that such structures are selective to the permeation of water molecules in particular[1,2]. It has been proposed that this property may endow nanoporous graphene and graphene sheets as candidates for desalination membranes. The process of diffusion through such membranes is expected to be mediated by adsorption mechanisms and confinement effects at the nanoscale. Computer simulation is an ideal tool for detailed study of the microscopic mechanism of diffusion in such systems. In this work we use steady-state Non-Equilibrium Molecular Dynamics simulations to study the diffusion of water through nanoporous graphene and layered functionalised graphene sheets. This method allows us to systematically investigate the selectivity of these materials and effectively evaluate their potential as reverse osmosis membranes.

References

[1] David Cohen-Tanugi and Jeffrey C. Grossman, *Nano Letters*, **12(7)**, 3602608 (2012).
[2] R. R. Nair, H. A. Wu, P. N. Jayaram, I. V. Grigorieva, A. K. Geim, *Science*, **335**, 442 (2012).