Computer Simulations of Graphene-Oxide-based Membranes for Water Desalination

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ABSTRACT

Non-Equilibrium Molecular Dynamics Simulations were performed to study water desalination through graphene-oxide multilayered membranes (fig. 1). Effects of the type of functionalization of the graphene oxide flakes and of the structural rigidity of the membranes in water permeability and ion rejection, were examined in detail. Description of microscopic mechanisms related to the membranes' performance such as hydrogen bonding, electrostatic interactions and concentration polarization allowed the assessment of the contribution of different factors involved in the desalination process. The performance of the membranes in water flux was found to surpass conventional membranes by 2-3 orders of magnitude, while functionalization was found to increase considerably ion rejection. The detail afforded by the present study provided new insight towards the design of membranes with optimized performance in water desalination.

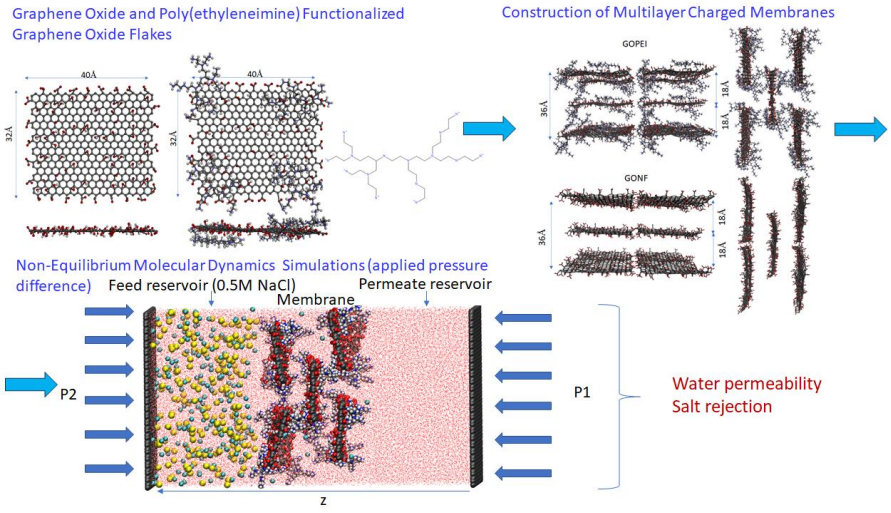

Figure 1: Multilayer Graphene Oxide Membrane Models for Water Desalination

KEYWORDS: Molecular Dynamics Simulations, Desalination, Graphene Oxide

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