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Graphene Based Materials as Novel Membranes for Water Desalination and Boron Separation

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Abstract : Desalination is one of the most employed approaches to supply water in the context of a rapidly growing global water shortage. However, the most popular water filtration method available is the reverse osmosis (RO) technique, still suffers from important drawbacks, such as a large energy demands and high process costs. In addition some serious limitations have been recently discovered, among them, the boron problem seems to have a critical meaning. Boron has been found to have a dual effect on the living systems on Earth and the difference between boron deficiency and boron toxicity levels is quite small. The aim of this project is to develop a new generation of RO membranes based on porous graphene or reduced graphene oxide (rGO) able to remove salts from seawater and to reduce boron concentrations in the permeate to the level that meets the drinking or process water requirements, by means of a theoretical approach based on density functional theory and classical molecular dynamics. Computer simulations have been employed to investigate the relationship between the atomic structure of nanoporous graphene or rGO monolayer and its membrane properties in RO applications (i.e. water permeability and resilience at RO pressures). In addition, an emphasis has been given to multilayer nanoporous rGO and rGO flakes based membranes. By means of non-equilibrium MD simulations, we investigated the water transport mechanism permeating through such multilayer membrane focusing on the effect of slit widths and sheet geometries. These simulations allowed us to establish the implications of these graphene based materials as promising membrane properties for desalination plants and as boron filtration.

Keywords : boron filtration, desalination, graphene membrane, reduced graphene oxide membrane
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