In this study, we investigate seawater filtering capability of carbon nanostructures. Carbon based nanomaterials such as carbon nanotubes (CNT) and graphene are good candidates for the desalination of seawater. Since they are hydrophobic, only the organic contaminants in the water adhere to carbon nanomaterials while water molecules pass through efficiently. Moreover, water filters made of carbon nanomaterials are expected to be reusable because of their high melting point (higher than 3000 °C). A simple heating method will evaporate all the contaminants in a carbon-based water filter, leaving the carbon structure intact. Moreover, during the heating process, defects and impurities generated during daily use of the filter are cured, recovering the original structure because of the heat treatment effect on the structure. Here, we employ atomistic simulations to evaluate the desalination capacity of different carbon-based nanomaterials. Also, the healing of defected carbon-carbon bonds under high temperatures is explored by running the atomistic desalination simulations at high temperatures. The cure of point defects as well as evaporation of organic contaminants are also investigated at different temperatures. The results obtained in this research study will provide another exciting solution to the global water scarcity since the nanostructured carbon-based seawater filter proposed here will be highly efficient and highly recyclable.

Keywords: Atomistic simulation, nanostructured carbon, reusable seawater filter