Desalination study of carbon nanotube with sidewall-nanohole via molecular dynamics simulation

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Reverse osmosis (RO) desalination is used for pure water obtained from sea water. Although various nanomaterials are now attempted for the application of desalination, their syntheses incorporating supporting materials are relatively difficult. However, single-walled CNT (SWNT) can make water molecules permeate through nanohole on the wall with self-supporting structure. Therefore, in this theoretical study, a new RO desalination system based on SWNTs with nanohole was studied by molecular dynamics simulation. To investigate the size effect of nanohole on permeating phenomena, we considered the CNTs with three sizes of nanoholes (i.e. diameter = 8 Å, 12 Å, and 15 Å), where dangling carbon atoms were passivated by hydrogen atoms and/or hydroxyl groups. Also, three types of SWNTs having different chiralities (i.e., (15,15) armchair, (18,12) chiral, and (26,0) zigzag) were modeled to investigate the mechanical properties related to the desalination process. The results demonstrated that SWNTs with 8 Å nanohole achieved 100 % salt rejection and water flux of 50 L/(m^2·h·atm), assuming the number density of nanohole as 4.63×10^{16} m^{-2}.