

Abstract

In this poster, we are seeking for holistic integrated multiscale model simulation suitable for sustainable nanotechnology solution. During the past ten years after nanotechnology has become a headline, there has been significant progress in the development of nanotechnology based solution in the area of water treatment, desalination, and reuse. One of the important issues to be addressed here is the design and optimization of nanostructured filters and membrane for distillation process to further enhance separation efficiency and water flux. Our focus in this poster is to provide an efficient tool based on lattice Boltzmann method and molecular/atomistic simulation hybridization capable of accurately predicting and optimizing membrane performances. The simulation tool we develop will eventually have capabilities of designing molecular level architecture of the membrane distillation materials.