No. 1516

Molecular Modeling of Reverse Osmosis Membranes by Investigating the Microscopic Behaviors of Compositions of Seawater

Ryo Nagumo

Nagoya Institute of Technology

Summary

Membrane fouling phenomena have been one of the significant challenges in the development of reverse osmosis membranes for seawater desalination. Many microscopic and macroscopic factors definitely influence the fouling properties of membrane surfaces. In particular, the hydrophilicity of the surfaces is one of the crucial factors of antifouling properties. In this study, molecular dynamics (MD) simulations were conducted to gain an insight into detailed mechanisms of the hydrophilicity. We investigated the hydration and association structures in the vicinity of repeat units of thermo-sensitive polymer gels, such as poly(*N*-*n*-propylacrylamide), poly(*N*-isopropylacrylamide), and poly(*N*-ethyl-*N*-methylacrylamide).

In the MD simulations, the temperatures were set to 270 K and 360 K, which are below and above their lower critical solution temperatures (LCSTs), respectively. Radial distribution functions (RDFs) between the repeat units and the surrounding water molecules were calculated to evaluate the hydration structures in the vicinity of the repeat units under 60wt% of water content. In addition, the RDFs between the repeat units were also calculated to assess the association structures on the corresponding water content. Our RDF data suggest that the difference in the LCSTs for the three types of polymers strongly correlates with the hydration structures and the association structures in the vicinity of the constituent nitrogen atoms in the amide groups. RDF calculations from MD simulations certainly contribute to the screening of crucial factors of varied properties, such as hydrophilicity and antifouling properties.