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# Assessment of Anti-Fouling Property of Membranes Using Computational Chemistry to Design Seawater Desalination and Salt Production Processes

Ryo Nagumo

Department of Materials Science and Engineering, Nagoya Institute of Technology

Summary

To develop reverse osmosis membranes for seawater desalination processes, it is significant to design and fabricate higher performance membrane materials. One of the key factors for the higher performance is the reduction of fouling phenomena, where suspended solids in seawater adhere to membrane surfaces. In this study, to promote the development of membrane materials with higher antifouling properties, interaction energies in the vicinity of the materials were evaluated by using molecular dynamics (MD) simulations. Particularly, hydrophilicity is one of the significant factors of antifouling properties and it is essential to measure and assess the hydrophilicities for polymer materials. A methodology to estimate the hydrophilicities using MD calculations was proposed and its accuracy was investigated.

Interaction energy profiles were calculated for a water molecule approaching each repeat unit of material to evaluate the hydrophilicities of polymer materials. In conducting MD simulations, intermolecular distances between a water molecule and a repeat unit were fixed. Energy profiles were assessed as functions of an intermolecular distance between a water molecule and a repeat unit, and minimum values of these profiles were determined.

Consequently, the minimum values were remarkably different between the types of material repeat units. When the values are smaller, the affinities between water molecules and repeat units are certainly higher, leading to higher hydrophilicity. On the other hand, larger minimum values suggest that the affinities are lower, probably resulting in higher hydrophobilicity. Our approach certainly leads to the highly efficient materials design of reverse osmosis membranes for seawater desalination processes.