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Material Design of Separation Membranes Using Computational Chemistry to Promote Salt Production and Marine Resources Utilization

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Summary

In the research and development of reverse osmosis membranes for seawater desalination, it is essential to improve membrane performances, such as water permeability, salt rejection, and antifouling properties. Aromatic polyamides have widely been used as a membrane material for desalination. The application of inorganic materials, such as zeolites and carbons, have recently been paid attention for a promising approach to fabricating novel high-performance reverse osmosis membranes. In this study, to evaluate antifouling properties of inorganic materials, the interaction energy profiles of an organic molecule approaching an inorganic material in aqueous solution were calculated by using molecular dynamics (MD) simulations. As a result, the profiles shows energetically stable minimum, suggesting that membrane fouling occurs on the surfaces.

Furthermore, we have focused on the hydrophilicity, because it is one of the significant factors of antifouling properties. The microscopic hydration behaviors in the vicinity of poly(*N*-isopropylacrylamide) (PNIPAAm), which is one of the most major thermo-responsive hydrogels, were investigated by using MD simulations. The temperatures were set at 270 K, 280 K, 290 K, 300 K, 320 K, 330 K, 340 K, and 350 K. Radial distribution functions (RDFs) between the oxygen atom in a NIPAAm repeat unit and the surrounding water molecules were analyzed for all the simulations. Consequently, the correlation between the maximum values of the RDFs and the temperatures were confirmed. As the temperature is higher, the maximum value becomes smaller. These approaches certainly contribute to the design of membrane materials for desalination processes.