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A Study on the Relationship between the Behavior of Water Molecules and Fouling Phenomena for the Materials Design of Reverse Osmosis Membranes

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Summary

To address the escalating global water crisis, the development of sustainable water treatment technologies is an urgent challenge. Our group has been conducting molecular-level investigations using molecular dynamics (MD) simulations to mitigate membrane fouling in reverse osmosis (RO) processes. While RO is a large-scale and widely established method for seawater desalination, attention is increasingly being drawn to directional solvent extraction (DSE) as a decentralized and small-scale complementary process. In response to this emerging trend, we have applied MD simulations to develop a modeling methodology aimed at rational solvent design for DSE applications.

In this study, we focused on binary mixtures of water and imidazolium-based ionic liquids, specifically [bmim][Tf_2N] and [emim][Tf_2N]. Three different water contents—50wt%, 70wt%, and 90wt%—were examined under temperature conditions of 300 K and 350 K. We performed MD simulations under each condition and calculated the radial distribution function (RDF), which characterizes microscopic interactions, as well as the second virial coefficient (B_2), which serves as an indicator of component miscibility.

Our analysis revealed that in binary mixtures with 90wt% water content, the ionic liquid and water exhibited increased dispersion at elevated temperatures. This trend was consistent with previously reported experimental findings. Given that water molecules exhibit significantly higher mobility than ionic liquids, it is presumed that systems with high water mole fractions—particularly the 90wt% case—yielded more reliable data due to improved sampling accuracy in the simulations. Further RDF analysis indicated that the hydration peak of water molecules around the anion was significantly closer to the anion than both the hydration peak around the cation and the cation–anion association peak. This suggests that the microscopic interactions between anions and water molecules play a crucial role in governing the dispersion and aggregation states within the system.

This research aims to establish a methodology for rational solvent selection in DSE processes and is expected to contribute to the advancement of sustainable water treatment technologies in the future.