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Development of a High-Speed Computational Chemistry Approach to Screening Reverse Osmosis Membrane Materials

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Summary

To enhance the antifouling property of reverse osmosis membranes for seawater desalination, it is essential to evaluate molecular interactions in the vicinity of materials at the atomistic level. In this study, molecular dynamics (MD) simulations are conducted to discuss the correlations between the molecular interactions and the antifouling properties. Our targets are the four trimers of carboxybetaine acrylamide materials, whose carbon numbers between the anionic groups and the cationic groups are one, two, three, and five. As a simplified foulant molecule, three organic solvent molecules are adopted: Ethylene glycol, 1,4-butanediol, and *tert*-butyl alcohol. Ternary mixture systems consisting of carboxybetaine trimers, water molecules, and organic solvent molecules are used as cubic simulation cells. By using the MD trajectory data at 298 K and at 1 bar, microscopic behavior is evaluated to calculate the ratio of the coordination number of water molecules over that of organic solvent molecules around the anionic groups of the constituent side chains of the carboxybetaine trimers.

Consequently, for the trimer/water/1,4-butanediol mixtures, the ratio of the coordination number reached the maximum value at the carbon number of 2. For the trimer/water/*tert*-butyl alcohol mixtures, the ratio reached the maximum value at the carbon number of 3. In a previous study, the antifouling property of poly(carboxybetaine acrylamide) was the highest at the carbon number of 3 and was the lowest at the carbon number of 5. That is, the antifouling property is possibly correlated with the ratio of coordination numbers of water molecules over that of organic solvent molecules around the anionic groups of the carboxybetain materials. Systematic investigations on the solvation structures for various types of organic solvent systems certainly contribute to validate the speculation.

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