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Theoretical Design of Extractants for the Efficient Separation of the Components of Seawater

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Summary

To separate the target component efficiently by adding the extractant to a liquid mixture, it is essential to investigate the phase separation of the target component. In this study, molecular dynamics simulations were conducted to evaluate the phase separation behavior at the atomistic levels. By developing an in-house simulation code, we evaluated the phase transition of *N*,*N*-dimethylaminoethyl methacrylate (DMAEMA) and the analog repeat unit in the aqueous solutions at 300 K. DMAEMA has a tertiary amine structure, whose terminal functional groups are methyl groups. For comparison, we also investigated the phase transition of a DMAEMA analog with a primary amine structure, whose terminal groups are hydrogen atoms.

We evaluated the phase separation in the deprotonated tertiary amine (DMAEMA)/water mixture and the protonated tertiary amine/water mixture, respectively. In the deprotonated tertiary amine/water mixture, we observed almost complete phase separation behavior, while the protonated tertiary amine are miscible. For the protonated primary amine/water/acetic acid mixture, radial distribution functions between the bicarbonate ions and the surrounding primary amines, the water molecules, and the acetic acid molecules were also calculated to evaluate the distribution of each component in the vicinity of the protonated hydrogen atoms in the primary amine structures. Consequently, the bicarbonate ions robustly bind to the protonated primary amines via strong ionic interactions. Furthermore, the bicarbonate ions tightly bind water molecules, suggesting that the bicarbonate ions serve as a mediator between the protonated amines and the water molecules. The bicarbonate ions certainly contribute to the hydrophilicity of the protonated amine structures.