Hydration structure of inorganic salt solutions at various concentrations: A molecular dynamics approach

Ayana Sato [a], Nanami Shima [b], Osamu Takahashi [c]

[a] *Department of Chemistry, Faculty of Science, Hiroshima Univ.*
[b] *Chemistry Program, Graduate School of Advanced Science and Engineering, Hiroshima Univ.*
[c] *Research Institute for Synchrotron Radiation Science, Hiroshima Univ.*

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Traditionally, water treatment membranes have been considered to function based on the molecular sieving principle. However, ion permeability measurements using a liquid crystal polymer membrane developed by Watanabe et al. [1] showed that $MgSO_4$ exhibited than NaCl. This suggests that the selective ion permeability is influenced not only by the ions themselves but also by the hydrogen bonding structure and stability of water molecules surrounding the ions.

To understand ion permeability, it is first necessary to examine the hydration structures of salt ions in detail. Therefore, we investigated the behavior of ions in salt solutions and the structure of water molecules.

Molecular dynamics (MD) simulations were performed for NaCl and $MgSO_4$ aqueous solutions at various concentrations up to saturation. The radial distribution function was calculated, several properties of the hydrogen bonding in solutions were analyzed. Furthermore, using structures obtained from the simulations, an X-ray emission spectroscopy (XES) spectrum calculation was performed on a 20-molecules cluster, which consisted of one water molecule selected randomly and the 19 surrounding water molecules.

First, the results of the radial distribution function confirmed that Mg^{2+} is closer to water than Na^+. Next, an analysis of the number of hydrogen bonds, their types, and their distribution revealed that, in the first hydration shell, all ions caused significant deviations from that of pure water. Comparing Mg^{2+} with Na^+, Mg^{2+} was found to be closer to water, with an overwhelming number of water molecules acting as hydrogen donors around it. In contrast, around Na^+, the water molecules were positioned farther away compared to Mg^{2+}, resulting in a dominance of water molecules acting as hydrogen acceptors.

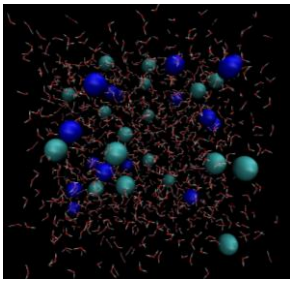

FIGURE 1. MD simulation of 1M NaCl solution

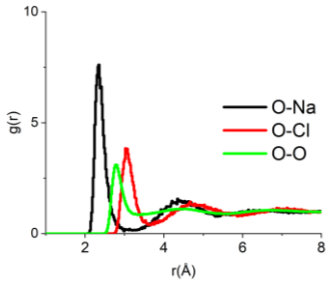

FIGURE 2. Radial distribution function of 1M NaCl solution

REFERENCES

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