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Molecular dynamics simulations of oil wettability of muscovite-NaCl solution interface

KOBAYASHI, Kazuya[1*] ; LIANG, Yunfeng[1] ; MATSUOKA, Toshifumi[1] ; NISHI, Naoya[1] ; SAKKA, Tetsuo[1]

[1]Graduate School of Engineering, Kyoto University

The investigations of the properties of mineral-electrolyte solution-oil interface are of importance for developments of resources and underground disposals of toxic wastes. The behavior of electrolytes at mineral-electrolyte solutions (e.g. formation of electric double layer) changes their properties. It is known that the wettability of mineral surface by oil in aqueous solutions depends on the concentration of the electrolytes. However, the fundamental relationship between the change in wettability and the behavior of electrolytes has not been revealed. Therefore, we applied molecular dynamics simulation, which provides nano-scale interfacial structure and dynamics of molecules, in order to investigate the mineral-electrolyte solution-oil interfacial structure and wettability. The muscovite, 3.0 mol/kg NaCl aqueous solution, and heptane or toluene were used as mineral, electrolyte solution, and oil, respectively. The simulations revealed that the adsorption of Na^+ at negatively charged muscovite surface decreases the interfacial tension at mineral-aqueous solution interface whereas negative adsorption of electrolytes increases the interfacial tension at oil-electrolyte solution interface for both the oil molecules. The changes in the two interfacial tensions alter the wettability of oil droplets. This research provides the fundamental knowledge for applications to enhanced oil recovery.

Keywords: Muscovite, Mineral-underground fluid interface, Wettability, Molecular dynamics