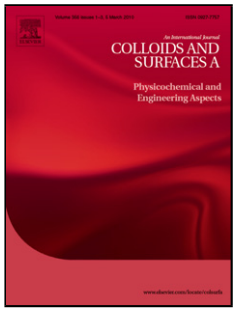

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Influence of Mg^{2+}, SO_4^{2-} and Na^+ ions of sea water in crude oil recovery: DFT and ab initio molecular dynamics simulations

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A detailed understanding of surface interaction between crude oil molecule and calcite can pave a way to explain several fundamental challenges of wettability alteration of calcite surface and hence provide a guidance for further enhancement of crude oil recovery. In the enhanced crude oil recovery stage, additives, Mg^{2+} and $SO_4{}^{2-}$ ions of sea water alter the relative wettability characteristics (from oil-wet to less oil-wet) of calcite surface that enhances the crude oil recovery. In this paper, we consider naphthenic acid is a model compound of crude oil molecule, perform Density Functional Theory (DFT) and ab initio molecular dynamics simulations and checking its relative binding energy (i.e. the binding energy difference between water and oil molecule) is an indication of relative wettability alteration of calcite surface. Ab initio molecular dynamcis simulations suggest that Mg^{2+} ion replaces Ca^{2+} of calcite and then SO_4^{2-} ion replaces CO_3^{2-} of calcite. The relative binding energy of oil molecule is larger on modified calcite.$MgSO_4$ surface than on pure calcite surface, providing an indication of less oil wet calcite surface. Ab initio moleculaur results also show that few Na^+ ions of sea water reach to the calcite surface as a precipitate and form Na naphthenates that make oil molecule more sticker (more oil-wet) to the rock surface. Combined study of DFT and ab initio molecular dynamics simulations can help to understand the surface interaction between oil molecule and calcite surface in aqueous sea water environment that has global impact on crude oil recovery from calcite oil reservoirs.

Keywords: Wettability alteration; Calcium; Magnesium; sulfate; Enhanced oil recovery, Density Functional Theory and ab initio molecular dynamcis