

Abstract Submitted  
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**Relative wettability alteration of calcite surfaces**<sup>1</sup> SANJAY PRABHAKAR, JIAN LIU, SOKRATES PANTELIDES, Vanderbilt University — Enhancement of crude oil recovery from calcite reservoirs remains a major challenge in the oil industry. Crude oil recovery can be enhanced by modifying the relative wettability of calcite reservoirs by injecting sea water. In this work, we consider acetic acid as a model component of crude oil and use the changes of adsorption energies of oil and water molecules induced by additives as a measure of relative wettability alteration of the calcite surface. More specifically, we investigate the influence of  $\text{Na}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{SO}_4^{2-}$  and  $\text{Cl}^-$  ions on the adsorption energies of water and acetic acid. It is expected that crude oil recovery is enhanced if the modified acetic acid molecule binds weaker than acetic acid. We use density functional theory calculations and show that the presence of  $\text{Na}^+$  ions reduces oil recovery whereas the presence of Mg and  $\text{SO}_4$  ions enhance oil recovery. Additionally, we propose a novel possibility of lifting two oil molecules by one  $\text{Mg}^{2+}$  ion, which yields enhanced oil recovery, as observed. We also found that Cl merely binds to the surface and has no effect on the adsorption energy of acetic acid, which means that Cl has no effect on oil recovery.

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Sanjay Prabhakar  
Vanderbilt University

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