MOLECULAR DYNAMICS SIMULATION OF SURFACTANT-DRIVEN WETTABILITY ALTERATION OF CALCIUM CARBONATE FOR ENHANCED OIL RECOVERY

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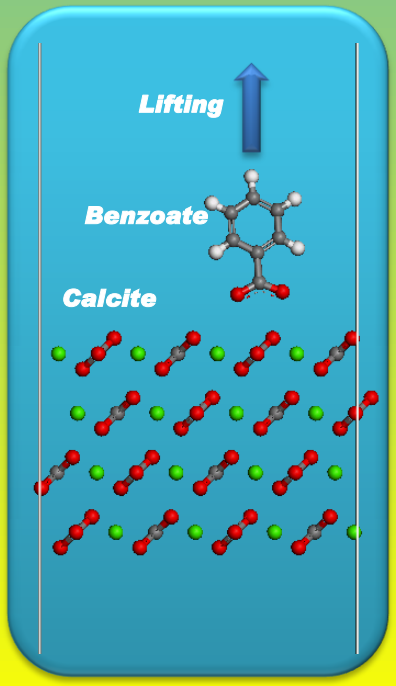
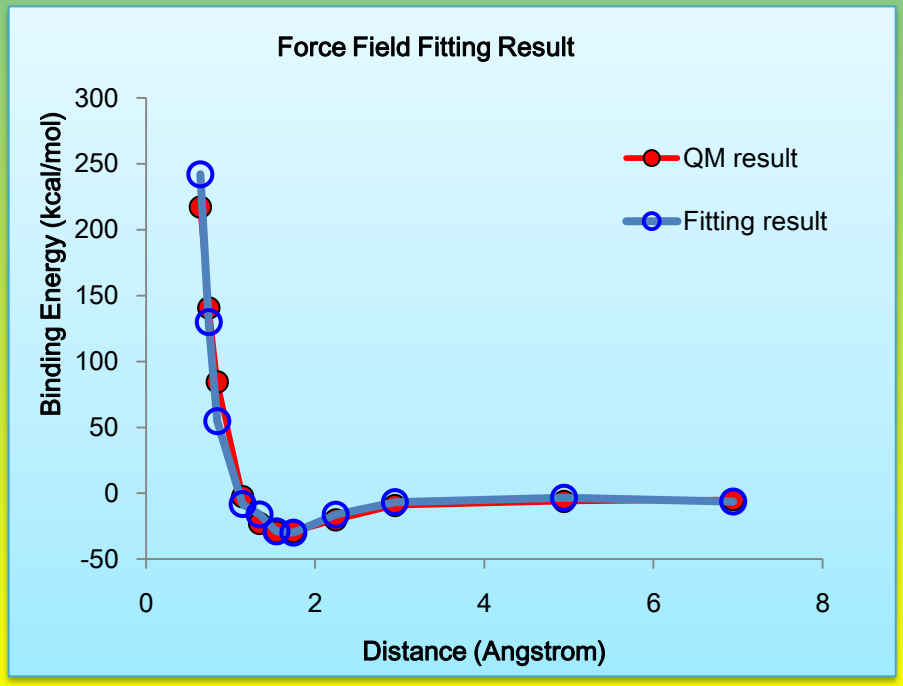
Since ~ 50 % of the petroleum reserves are found in carbonate reservoirs and the average oil recovery from carbonate reservoirs through the water flooding method is often less than 30 %, the development of more efficient and productive technology for enhanced oil recovery (EOR) is very essential to fully utilize our energy resources as well as to reduce the energy consumption in producing a unit volume of petroleum from the reservoirs. In order to enhance the oil recovery from carbonate reservoirs, it is desirable to alter the wettability of the carbonate surface using surfactants from the oil-wet surface to the water-wet surface. However, the detailed mechanism of the wettability alteration has not been understood completely at molecular level, which should be a critical requisite in developing better EOR technology. Thus, we are investigating the molecular mechanisms of the surfactant-mediated wettability alteration on the carbonate surface.

Benzoate is the carboxylate existing in crude oil. This compound is absorbed and dominantly influences the wettability of carbonate surface. We have successfully developed new Force Field parameters in order to investigate the adsorption/desorption of benzoate molecules from the calcite surface. The figure on the right demonstrates the applied method to measure the adsorption energy in quantum mechanics calculation. Based on this energy curve, we created new force field parameters to specifically describe the interaction between benzoate molecule and calcite surface.





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