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Adsorption Behavior and Mechanism of Illite Surface Under the Action of Different Surfactants

Authors : Sun Xiuxia

Abstract : As a critical mineral component of shale, illite is essential in oil exploration and development due to its surface hydration characteristics and action mechanism. This paper, starting from the perspective of the molecular structure of organic matter, uses molecular dynamics simulation technology to deeply explore the interaction mechanism between organic molecules and the illite surface. In the study, we thoroughly considered the forces such as van der Waals force, electrostatic force, and steric hindrance and constructed an illite crystal model covering C8-C18 modifiers. Subsequently, we systematically analyzed surfactants' adsorption behavior and hydration characteristics with different alkyl chain numbers, lengths, and concentrations on the illite surface. The simulation results show that surfactant molecules with shorter alkyl chains present a lateral monolayer or inclined double-layer arrangement on the illite surface, and these two arrangements may coexist under different concentration conditions. In addition, with the increase in the number of alkyl chains, the interlayer spacing of illite increases significantly. In contrast, the change in alkyl chain length has a limited effect on surface properties. It is worth noting that the change in functional group structure has a particularly significant effect on the wettability of the illite surface, and its influence even exceeds the change in the alkyl chain structure. This discovery gives us a different perspective on understanding and regulating the wetting properties. The results obtained are consistent with the XRD analysis and wettability experimental data in this paper, further confirming the reliability of the research conclusions. This study deepened our understanding of illite's hydration characteristics and mechanism. We provided new ideas and directions for the molecular design and application development of oilfield chemicals.

Keywords : illite, adsorption, wettability, hydration, surfactant
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