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Water Thin Films on Kaolinite Gibbsite and Edge Surfaces and Their Effects on Surface Wettability in Relation to Geological Carbon Sequestration

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Geological carbon sequestration (GCS) in subsurface media is one of promising approaches to alleviate excessive CO₂ emission [1], while saline aquifers are ideal GCS sites [2, 3]. Generally, four trapping mechanisms including: structural/stratigraphic trapping, residual trapping, solubility trapping and mineral trapping are proposed for GCS in saline aquifers [4, 5]. Among them, structural trapping plays a dominant role in the early stage of GCS, during which CO₂ can be sealed in porous media thanks to the capillary pressure between CO₂ phase and water phase [6, 7], which is dependent on CO₂-water-rock contact angle. It is reported that clay minerals such as kaolinite, account for a large proportion in caprocks. Thus, the knowledge about CO₂-water-kaolinite contact angle is of great importance for CO₂ structural trapping.

Kaolinite is a typical 1:1 type clay, consisting of one tetrahedral sheet and one octahedral sheet, which are known as siloxane and gibbsite surfaces, respectively [8]. Previous experimental and computer simulation studies [9-12] have shown that kaolinite gibbsite surface is hydrophilic, while siloxane surface is moderately hydrophobic [12]. Although these studies offer general understanding about CO₂-water-kaolinite contact angle, they have notable limitations. For example, it is extremely challenging to distinguish kaolinite surfaces in experiments, while the kaolinite surfaces used in experiments are often coated with quartz [11] and soil [9], and sample qualities are highly dependent on their preparation processes [13].

While CO₂-water-kaolinite contact angle on two kaolinite basal (gibbsite and siloxane) surfaces has been heavily studied [14], the contact angle on kaolinite edge surface remains unclear. Bickmore et al. [15] reported that the ratio of kaolinite edge surface area to total surface area can be up to ~50%. The water-edge surface interactions, interfacial water structures, and edge surface wettability still remain unknown. Kaolinite edge surface is not atomically flat [16, 17], while surface wettability is also dependent on surface roughness [18]. To the best of our knowledge, kaolinite edge surface wettability in CO₂-water-kaolinite system has not been reported yet.

Thus, in this work, we use molecular dynamics simulations to investigate kaolinite gibbsite and edge surfaces wettability in CO₂-water-kaolinite systems and elucidate the effect of interfacial water structures at a typical GCS condition (330 K and 200 bar). We find that both gibbsite and edge surfaces are strongly water-wet, while CO₂-water-kaolinite contact angle (i.e., 180°) on edge surface is even larger than that of gibbsite surface (i.e., 153°). Due to strong surface atomistic heterogeneity, water thin films with multi-layered hydration structures emerge on edge surface by forming complex hydrogen bonding networks and deplete CO₂ molecules from the surface. On the other hand, in the presence of CO₂ molecules, water thin films on gibbsite surface consist of single water adsorption layer.

Collectively, our work provides important insights into the dependence of water thin films and interfacial water structures on surface heterogeneity and their effects on surface wettability in CO₂-water-kaolinite systems, enhancing fundamental understanding about CO₂ structural trapping for GCS.

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