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Molecular Dynamics Study of Carbonated Water Confined in Nano Slit Illite Pore: Effect of the Layer Charge

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Wettability is an essential property in terms of structural trapping, which is considered to be the primary mechanism of CO2 geological storage [ref. 1]. Illite, a dioctahedral 2:1 phyllosilicate of common occurrence in soils and sedimentary rocks, is one of the main components of the caprock [ref. 1]. In this study, we focused on the interface of carbonated water and illite. This interfacial system is expected to occur when CO2 dissolution has progressed for some time after injection, or when CO2-dissolved water is injected. It is known that water forms a stable adsorption film [e.g., ref. 2-4] because water molecules interact strongly with the clay mineral surface. However, few studies have been performed to investigate the effect of the layer charge. How the water film is affected by the CO2 concentration and the behavior of CO2 is still not well understood.

This study investigated the interfacial structure and dynamics of carbonated water by using molecular dynamics simulations for illite slit systems with different layer charges.

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Japan

References

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Time Block Preference

Participation

Online

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