Contribution ID: **96** Type: **Poster Presentation**

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

Monday, 30 May 2022 09:40 (1h 10m)

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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Country

Japan

References

[1] Iglauer, S., Pentland, C. H., & Busch, A. (2015). CO2 wettability of seal and reservoir rocks and the implications for carbon geo-sequestration. Water Resources Research, 51(1), 729-774.
[2] Sakuma, H., & Kawamura, K. (2009). Structure and dynamics of water on muscovite mica surfaces. Geochimica et Cosmochimica Acta, 73(14), 4100-4110.
[3] Shiga, M., Aichi, M., Sorai, M., & Morishita, T. (2021). Structure and Dynamics of Interfacial Water on Muscovite Surface under Different Temperature Conditions (298 K to 673 K): Molecular Dynamics Investigation. Water, 13(9), 1320.
[4] Shiga, M., Morishita, T., Aichi, M., & Sorai, M. (2021). Effect of Surface Coverage of Water Molecules on Methane Adsorption on Muscovite and Pyrophyllite: Molecular Dynamics Study. Energy & Fuels.

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Online

Primary author: Dr SHIGA, Masashige (Geological Survey of Japan, National Institute of Advanced Industrial Science and Technology (AIST))

Presenter: Dr SHIGA, Masashige (Geological Survey of Japan, National Institute of Advanced Industrial Science and Technology (AIST))

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