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Methane adsorption on Silica-Kaolinite interface for shale gas application: A theoretical study

Thursday, 3 June 2021 20:00 (1 hour)

Methane mostly makes up the constituent of shale gas and it is currently being exploited in fulfilling the world's energy demands [1]. Molecular simulation techniques including Density Functional Theory (DFT) and Molecular Dynamics (MD) techniques are employed to understand methane transport in the pores at typical reservoir conditions [2]. To simulate the shale model which in reality is made up of clay and quartz-like material, an interface is created from the pure surfaces of silica (quartz) and kaolinite (clay) [3,4]. The simulations revealed that the interface is formed by a chemical bond between a silicon atom from the silica surface and two oxygen atoms from the kaolinite surface. The adsorption of methane was studied at three different positions on the Silica-Kaolinite interface namely, silica-dominated region, interface region, and kaolinite-dominated region. The mode of adsorption of methane irrespective of its position on the interface was found to be physisorption [5]. However, methane has stronger adsorption on the kaolinite region than the silica region. This results provides insight at the molecular level of methane interaction with a silica-kaolinite interface which will be useful in shale reservoir application particularly in estimating the original gas in place.

Time Block Preference

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

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