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Molecular competitive adsorption mechanism of methane and helium in illite of shale gas reservoirs through molecular simulation

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Shale gas in southern China possesses helium with industrial value (up to 2200ppm), and the helium concentration increases with the increase of age and burial depth of shales[1]. However, conventional perspective holds that shales can generate amounts of hydrocarbon gases which would dilute helium to sub-economic levels[2]. Here, we perform the Grand Canonical Monte Carlo simulation of the molecular competitive adsorption behaviors of methane and helium in illite nanopores to uncover the helium accumulation mechanism in shale gas reservoirs. The simulation condition includes the pore with diameter of 2 nm, helium concentration of 0.1%, 0.5%, and 1.0%, pressure for 0.1 MPa up to 200 MPa and temperature at 318.15, 368.15, and 418.15 K. The isothermal adsorption simulation result show that the absorption amounts of methane, helium and total gas increase with the increase of pressure and decrease with the increase of temperature. At the same temperature, the total absorption isotherms with different helium concentration are almost coincident (Fig. 1). The preferential selectivity indicator ($S_{CH4/He}$) have similar characteristics (Fig. 2), which shows that these two parameters are hardly affected by the helium concentration when it is extremely low (≤1.0%). The value of $S_{CH4/He}$ is almost all less than 1.0, which means that the adsorption capacity of helium in illite is stronger than methane. In addition, the $S_{CH4/He}$ value decrease with the increase of temperature (Fig. 2), which indicates that high temperature would enhance the competitive adsorption capacity of helium in illite. In conclusion, helium is preferentially absorbed in illite under the geological conditions, which contributes to helium accumulation in the shale gas reservoirs. Moreover, with the increase of burial depth of a set of shale, although the adsorption amounts of helium, methane and total gas will decrease, the concentration of adsorbed helium will increase.

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Fig. 2 Variations of S(CH_4/He) with helium concentration of 0.1%, 0.5%, and 1.0% at 318.15, 368.15, and 418.15K.

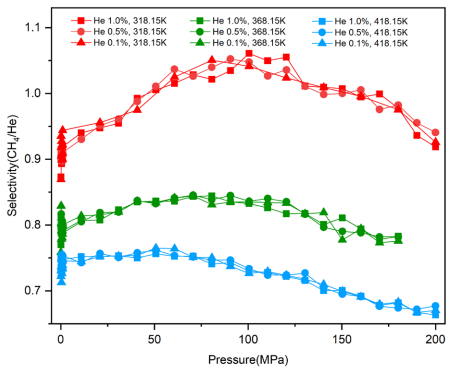

Fig. 1 The total gases adsorption isotherms with helium concentration of 0.1%, 0.5%, and 1.0% at 318.15, 368.15 and 418.15K.