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Physical Experiments and Mechanism Study on the Occurrence State of Hydrogen in Clay Minerals

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Natural hydrogen, discovered in diverse geological settings, has sparked global interest, yet its subsurface storage mechanisms remain poorly understood. This study investigates hydrogen adsorption behaviors in clay minerals and rock samples formed by the combination of clay and other minerals to elucidate retention mechanisms. Systematic hydrogen adsorption experiments on six pure clay minerals (montmorillonite, chlorite, sepiolite, palygorskite, kaolinite, illite) were conducted under varied temperatures (0–75°C) and pressures (0–18 MPa), complemented by density functional theory (DFT) and grand canonical Monte Carlo (GCMC) simulations. Results reveal significant adsorption differences: Sepiolite and palygorskite showed a higher excess adsorption capacity for hydrogen gas, far exceeding that of montmorillonite and chlorite, while illite and kaolinite almost did not adsorb hydrogen gas. This significant difference in adsorption capacity is mainly attributed to their unique pore structures, especially the differences in specific surface area and micro- and mesopore volumes. More complex pore structures and larger specific surface areas can provide more adsorption sites for hydrogen molecules. Sepiolite and palygorskite can adsorb hydrogen gas both in the bulk and on the external surface, while montmorillonite and chlorite mainly adsorb hydrogen gas on the external surface. Adsorption capacity inversely correlates with temperature and positively with pressure. For SK2 well samples in Songliao Basin, hydrogen enrichment in mudstones of Dengloukou and Yingcheng Formations is adsorption-dominated, controlled by meso/microporosity and surface chemistry, whereas sandstones store hydrogen as free gas within structural/diagenetic traps. This study establishes a model where crust-mantle derived hydrogen migrates via faults and accumulates in clay-rich strata, constrained by pore architecture and capillary sealing. The findings advance the understanding of hydrogen occurrence in terrestrial basins and provide critical insights for targeting hydrogen reservoirs, integrating mineralogical characterization with multiscale simulations to bridge molecular-scale mechanisms and reservoir-scale prediction.