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High-pressure Hydrogen Adsorption in Clay Minerals: Insights on Natural Hydrogen Exploration

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Natural hydrogen has been widely detected in many environments. However, up to date, the knowledge about the occurrence of hydrogen in the geological formation is very limited. Clay minerals with large adsorption capacities due to their huge specific surface area are widely distributed in the subsurface. In order to find whether the hydrogen can be adsorbed on the clay minerals, 6 types of clay minerals (montmorillonite, chlorite, sepiolite, palygorskite, kaolinite and illite) were used for the hydrogen adsorption analysis at various temperatures (0, 25, 45, and 75 °C) and pressures (up to 18 MPa). In addition, multi-scale simulations via density functional theory (DFT) and grand canonical Monte Carlo (GCMC) were carried out to further explore the hydrogen adsorption mechanism of clay minerals in bulk phase. The results show that the excess adsorption capacities of sepiolite and palygorskite are much higher than those of montmorillonite and chlorite, and the excess adsorption capacities of illite and kaolinite are very low, nearly reaching the detection limit. The variation of hydrogen adsorption capacity (HAC) in different clays is attributed to the difference in their pore structures (i.e., specific surface area). A more complex pore structure and a larger specific surface area could provide more sorption sites for hydrogen molecules. HAC increases with pressure and decreases with temperature irrespective of the clay mineral types. This study highlights the features of hydrogen adsorption in clay minerals, contributes to a better understanding of natural hydrogen occurrence and storage in the subsurface, providing the potential application for geological hydrogen exploration.