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Molecular Insights into Caprock Integrity of Subsurface Hydrogen Storage: Perspective on Hydrogen-induced Swelling and Mechanical Response

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The integrity of caprocks in subsurface hydrogen storage is crucial for preventing leakage and ensuring long-term safety. A significant yet often overlooked factor in caprock integrity is hydrogen-induced swelling in clay minerals. When hydrogen molecules are intercalated into the interlayer nano-space of clays, they can induce changes in the structural properties, such as the expansion or shrinkage of interlayer pores, which in turn can impact the mechanical response of the caprock. Using Molecular Dynamics simulations, we investigate how the intercalation of hydrogen within dry, partially to fully saturated of clay mineral interlayer spaces affect swelling behaviour and mechanical properties. In this talk, I will present our recent findings, providing new insights into the molecular mechanisms of this phenomenon and its implications for caprock integrity in subsurface hydrogen storage.

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References

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