S6-2.2

Investigation into Interlayer Water Structure in Na^{+}- and Ca^{2+}-Montmorillonite: A Molecular Dynamics Study

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Swelling clays play significant roles in current industry. Molecular dynamics simulations have been performed to investigate the swelling properties, hydration behaviour and mobility of interlayer molecules of Na^{+}- and Ca^{2+}-montmorillonites. More specifically, to characterize the structure and energetics of Na^{+} and Ca^{2+} adsorption as functions of water content; the relationships between the coordination environments of clay surface–interlayer water–exchangeable cations; the influence of cation hydration energy on the dynamics and swelling mechanism of clays; and the influence of charge distribution on all of the above. Establishing an understanding of these clay/water systems is viewed as a sensible foundation for the more complex systems.