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Influence of layer charge location and inter-layer cations on swelling properties of mixed layer Illite-Montmorillonite

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Swelling of clay minerals play an important role in many fields including gas and oil industry and 〖CO〗_2 sequestration. More than 60 percent of sedimentary samples in the US are of different types of mixed layer clays. We used molecular dynamics simulations to investigate the effects of layer charge location, interlayer cations (K^+ and 〖Na〗^+) and their concentration ratio on swelling of mixed layer Illite-Montmorillonite. Illite-Montmorillonite mixed layer consists of Illite-Montmorillonite and Montmorillonite-Montmorillonite interlayers. For all of the cases of this study, d-spacing was measured as a function of water content.
For Na-montmorillonite model with layer charge concentrated in the octahedral sheet, weak ion–surface interaction results in fully hydrated ions and therefore more swelling. This is in good agreement with the previous experimental and computational findings. However, in the asymmetric interlayer of mixed layer Na-Illite-Montmorillonite, the Illite side with stronger surface-ion interactions results in a considerable cation concentration near the Illite surface. This limits hydration of cations and therefore controls swelling in mixed layer clays compared to the pure Montmorillonite interlayer. In addition, further inhibition of swelling from that of Na-mixed layer can be reached with increasing K^+ to 〖Na〗^+ ratio in the interlayer. However, it was shown that increasing K^+ fraction above 0.7 is not strongly felt by the mixed layer clays. Moreover, Clay hydration enthalpies, interlayer atomic density profiles and radial distribution functions are consistent with the swelling results in all cases.

References

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