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Dynamic properties of nano-pore water in 2:1 clay minerals: Effects of interlayer cations and isomorphic substitutions

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Clay minerals like kaolin and smectite are among the world's most valuable industrial minerals. They play considerable role in geotechnical, agricultural, and pharmaceutical applications. The static and dynamic properties of a confined fluid between structured clay surfaces are different from their bulk properties. The difference is related to complex nature of interatomic forces between negatively charged clay sheets, polar water molecules, and interlayer cations in nano-pores. Molecular dynamics is utilized to study the correlated effect of hydration state, interlayer cation size and charge, and molecular structure of clay minerals. Interlayer structure, mobility, activation energies, and density spectra of vibrational modes of water molecules are investigated at different hydration levels from 0 to 500 mg_{water}/g_{clay} in 2:1 clay minerals. Confinement of water molecules between clay sheets increases the activation energy in the interlayer compared to the bulk state. With increasing the charge density of clay surface and hydration energy of interlayer cations, the mobility of water molecules decreases. At higher water contents (more than 300 mg_{water}/g_{clay}) vibrational spectra of interlayer water come close to the bulk water, while the variation in lower water contents is affected not only by charge density of clay plates, but also by location of isomorphic substitutions.

References

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