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Water dynamics in a saponite: coupling molecular dynamics and NSE experiments

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Clays are porous lamellar materials with remarkable properties of adsorption and retention, which make them good candidates for environmental applications such as water pollution control or waste storage (radioactive, CO₂). The retention properties of the mobile species are strongly influenced by the behavior of water in the medium.

On one hand, classical molecular simulations make it possible to describe and quantify the diffusion processes in water/clay systems, as soon as the interactions between the atoms are well defined. On the other hand, QENS experiments provide valuable information on water dynamics in this systems, as soon as a reliable model of analysis is found. I will show on an oriented sample of hydrated saponite how the modeling/NSE experiment coupling allows 1) to find the right model of analysis, 1) to interpret the experiments and their evolution with temperature 3) to define the limit of validity of the simulations.

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