A fresh molecular look at calcite-brine confined interfaces: hydrogen bond network and modelling NMR

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Calcite-brine interfacial properties are crucial for understanding geological processes such as biomineralization and oil exploration. Under confinement, these properties can change and modify petrophysical and chemical physics properties. Nuclear magnetic resonance (NMR) relaxation is an effective technique for probing the dynamics of proton-bearing fluids in porous. In addition, the water dynamical properties are directly related to the hydrogen bond network (HBN) structure. In this work, we use fully atomistic molecular dynamics simulations to perform a HBN graph analysis and calculate the NMR T2 relaxation time for pure water and API brine confined in calcite (104) slit pores (Mutisya et al, J. Phys. Chem. C, 2017, 121,6674). Specifically, we have investigated the effect of salt ions (Na, Cl, Ca) and water-calcite interactions (layer by layer analysis) and geometric confinement – varying pore sizes (6 to 1 nm) The water dynamics and HBN structure are mainly affected near (1nm) the calcite surface due the strong fluid/surface interaction. Under confinement, the diffusion and reorientation of water molecules are slow. For calcite pores, our results indicate that the two kinds of dynamics are uncorrelated. The presence of ions further slowdown the diffusion coefficient and rotational correlation time, which can be understood with the formation of a more continuous HBN structures.

Fig. NMR and HBN analysis of calcite-brine interfaces.