

Structure and Dynamics of water in confined pores - dehydration effects in natural zeolites

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The nature of water within the nanopores of zeolites is far from being liquid. However, the fluidity of this water is critical in not only forming these materials (naturally and synthetically) but also as the transport medium for ion exchange. Our work in simulating (computationally) the formation and properties of these materials requires careful parameterisation and as part of this work we have undertaken parallel experimental work to validate some of our methods and results. Here we will discuss the specific case of the zeolite Goosecreekite and its dehydration. The availability of a combination of X-ray diffraction and Raman spectroscopy at the SNBL allowed us to probe the dynamics and structure of this material during dehydration, revealing metastable phases with changes in water dynamics, which we have subsequently been able to simulate.