Dynamics of Confined Water in Carbon Nanohorns And Porous Magnesium Carbonate

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We have studied the dynamics of water confined in carbon nanohorns and in a magnesium carbonate material, upsalite, using the neutron backscattering spectrometer SPHERES at MLZ, Garching.[1,2] Carbon nanohorns are analogous to carbon nanotubes except for different topology thus providing more heterogeneous confining environment. Upsalite, on the other hand, is a novel mesoporous material with exceptional water adsorption properties. In the case of carbon nanohorns, we studied the acquired spectra over the whole accessible q range in contrast to what seems the contemporary standard procedure. A rigorous analysis of the q and temperature dependencies of the relaxation times revealed a transition from local dynamics to more long range displacements near 225 K. Contradicting the fragile-to-strong crossover hypothesis, the transition was not thermodynamical, as shown by the q dependency of the transition temperature. Above around 250 K, the quasielastic line broadened to a degree which prevented unambiguous fitting in the time window of the spectrometer. However, a weak Lorentzian with temperature independent width was present at these temperatures. This line was attributed to functional groups at the surface of the nanohorns. On the other hand, water in upsalite showed different behaviour to nanohorns and other common matrix material, such as MCM-41. The acquired spectra were not stretched but could be fitted with a single Lorentzian plus a delta line over a much broader temperature range, up to 360 K. At low temperatures, degeneracy between the delta line and the Lorentzian rendered observation of the usual super-Arrhenius behaviour of relaxation time impossible. Surprisingly, the dynamics did not escape the narrow time window of SPHERES at high temperatures. The slow dynamics even above the melting point of water were attributed to unusually high amount of bound water and partial crystallization of the matrix material during the experiment.

References:

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