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On The Water Dynamics inside Carbon Nanotubes: NMR Spectroscopy and MD Simulation Techniques

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Extended Abstract

Several theoretical studies using molecular dynamics MD simulations showed an enhancement of water dynamics inside hydrophobic channels and reported a peak of the liquid self-diffusion coefficient at certain carbon nanotube sizes. However, experimental confirmation of this size-dependent liquid-dynamics was so far lacking. Here, we report two-dimensional NMR spectroscopy diffusion –relaxation 2D D-T_2, relaxation-relaxation 2D T_1-T_2 measurements as well as MD simulations of water in carbon nanotubes (CNTs) of different diameters (1.1 nm to 6nm) in the temperature range of 305-265 K. These NMR methods provide unique ways to distinguish water in the interior of CNTs from bulk water and water adsorbed on the external surface of the CNTs. Experiments show that water inside CNTs is further resolved into two components with different diffusion coefficient (D) values; water in proximity with the CNT walls, and water along the CNT axis. We were able to confirm experimentally, for the first time, a favorable diameter range in which maximum water dynamics occur as predicted by MD simulation works.

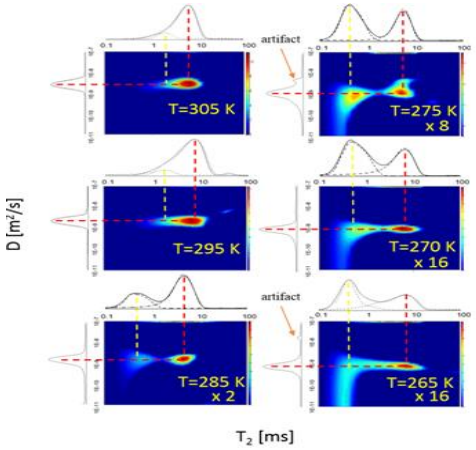

Figure 1: Two Dimensional NMR Diffusion-relaxation (2D NMR D-T_2) of water inside single walled Carbon nanotubes, at different temperatures.

References

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