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Diffusive Dynamics of Water inside Hydrophobic Carbon Micropores Studied by Neutron Spectroscopy and MD Simulation SOULEYMANE DIALLO, LUKAS VLCEK, EUGENE MAMONTOV, JONG KEUM, JIHUA CHEN, Oak Ridge National Laboratory, JOSEPH HAYES, American Technical Trading, DAVID WESOLOWSKI, ARIEL CHIALVO, Oak Ridge National Laboratory — Using neutron scattering, we have investigated the ambient pressure diffusive dynamics of water in microporous Kynol^{TM} ACF-10 (with average micropore size of $\sim$11.6 Å) from temperature $T = 280$ K in its stable liquid state down to $T = 230$ K into the metastable supercooled phase. The observed characteristic relaxation times and diffusion coefficients are found to be respectively higher and lower than those in bulk water, indicating a slowing down of the water mobility with decreasing temperature. Comparison between the experimental observations and complementary molecular dynamics simulations of a model system, in which we studied the diffusion of water within the 12 Å gap of two parallel graphene sheets will be presented.

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