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Water confined in carbon nanotubes: Magnetic response and proton chemical shieldings[1] PATRICK HUANG, ERIC SCHWEGLER, Physics and Life Sciences Division, Lawrence Livermore National Laboratory, GIULIA GALLI, Department of Chemistry, University of California, Davis — Carbon nanotubes (CNT) provide a well-defined environment for the study of confined water, whose behavior can differ markedly from bulk water. The application of nuclear magnetic resonance (NMR) to probe the local water structure and dynamics in these cases is hindered by ambiguities in the interpretation of the NMR spectra. We employ linear response theory to evaluate the ^{1}H chemical shieldings of liquid water in semiconducting CNTs, where the electronic structure is derived from density functional theory with periodic boundary conditions. The shieldings are sampled from trajectories generated via first-principles molecular dynamics simulations at ambient conditions, for water in CNTs with diameters $d = 11$ Å and 14.9 Å. We find a large (~ -23 ppm) *upfield* shift relative to bulk liquid water, which is a consequence of strongly anisotropic magnetic fields induced in the CNT by the applied magnetic field.

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