Abstract Submitted
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Water in nanoscale confinement: Insights into structure, dynamics, and ^{1}H-NMR chemical shifts from first-principles theory[1] PATRICK HUANG, ERIC SCHWEGLER, Physical Sciences Division, Lawrence Livermore National Laboratory, GIULIA GALLI, Department of Chemistry, University of California, Davis — The properties of water confined to nanoscale dimensions can differ markedly from bulk water. Numerous studies of confined water focus on water in carbon nanotubes (CNTs), because CNTs provide a uniform environment with a well-defined geometry and chemical composition. However, the behavior of water in CNTs remains controversial. Here, we apply first-principles density functional theory (DFT) to study the structure and dynamics of water in CNTs, and relate our microscopic picture to experimentally-accessible observables. One such observable is ^{1}H-NMR, a sensitive probe of atomic-scale structure and dynamics. While empirical procedures to relate chemical shifts to structure are known for organic molecules, analysis of NMR spectra of solids and liquids requires more sophisticated approaches. We evaluate chemical shifts of water in CNTs within periodic DFT, and relate our findings to experimental ^{1}H-NMR measurements.

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