

Abstract Submitted  
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**Structural and dynamical properties of water in hydrophobic confinement, as probed by *ab-initio* molecular dynamics.** GIANCARLO CICERO, Politecnico of Torino, Torino, Italy, JEFFREY C. GROSSMAN, Center of Integrated Nanomechanical Systems, University of California, Berkeley, ERIC SCHWEGLER, LLNL, Livermore, CA, GALLI GIULIA, University of California, Davis, CA — Unraveling the microscopic properties of water confined in small channels will help understand fluid flow and transport at the nanoscale, and will shed light on the solvation of biomolecules. To date most of the properties of confined water are poorly understood and, in many cases, controversial. We present a first principles computational study of prototype systems —water confined between graphene sheets and inside carbon nanotubes— which have received widespread experimental attention and for which, however, such basic questions as diffusion at the nanoscale, and characteristics of the hydrogen bonded network remain unanswered. Our simulations show that the liquid density substantially increases at the water/surface interface, and that water diffusion is faster in highly confined structures, due to a decrease of the dipole moment in interfacial water molecules and correspondingly a decrease in H-bond network strength. We propose that many effects attributed to confinement in the past are actually interfacial effects due to subtle electronic structure rearrangements, and that these are amenable to vibrational and x-ray absorption spectroscopy investigations.

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