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**First principles spectroscopy of confined water.** MANU SHARMA, GIULIA GALLI, Department of Chemistry, University of California, Davis — In order to characterize the changes in hydrogen bonding in water confined at the nanoscale, and to understand the effect of the interface between water and the confining medium, we carried out a spectroscopic investigation using first principles calculations. In particular, we computed the infrared (IR) spectrum of liquid water confined between two sheets of graphite. While the far IR region of the spectrum contains features characterizing the H-bond dynamics in water, we find a significant overlap of this region with the vibrational modes of graphite. We also find modes in the near IR region $\sim$2500 cm$^{-1}$, associated to the OH stretching mode, which while present in the kinematical (power) spectrum are absent from the computed IR spectrum. We demonstrate that these modes arise due to a dynamical charge transfer between water molecules and the p – orbitals of the graphite surface.

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