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A non-local Density Functional Theory for water adsorbed in nanoporous materials.

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Water confined in nanoporous materials has focused many attentions due to its vast number of technical applications and scientific fields such as geosciences, biology, catalysts, gas separation, etc [1,2 Indeed, confinement of water in nanopores affects its thermodynamic properties such as its density, its freezing temperature, the crystal structure, etc. For some years now, porosimeter manufacturers have been integrating the ability to perform high-precision measurements of adsorption of vapors at low pressure, including water. In parallel, thermoporosimetry appears to be a good alternative - or at least a good complementary technique - to gas porosimetry and mercury intrusion, especially for the investigation of the samples that can be destroyed in drying process [3]. The common features between water vapor sorption analysis and thermoporosimetry is that a reliable model of water adsorption inside nanopores is necessary to interpret the experimental data and try to obtain structural information of the porous materials from these measurements. In this work, we present a new NLDFT framework for confined water based on the general formulation of Wertheim's thermodynamic perturbation theory [4] and the statistical associating fluid theory [4]. The resulting model can be employed to determine the microscopic structure of inhomogeneous water in pores of arbitrary 3D geometry. It is first used to compute the density distribution, adsorbed amount, hydrogen bonding, pore pressure, adsorption-desorption behavior at pore scale. Then, the information is upscaled to compute water adsorption isotherms in microporous adsorbents and compare them with experimental data.

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