18. Themodynamic and Dynamic anomalies in water in porous media

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Water exhibits thermodynamic, dynamic and structural anomalous properties when compared with other substances. While most liquids contract upon cooling, water expands below T = 4ºC at ambient pressure, which characterize the densit anomaly. Recently, confined water has been receiving a lot of attention due the its applications in industrial and biological systems. In this work, we study the effects of a confinement of a water-like model in random porous media by two different approaches. First, we employ molecular dynamics simulation in the canonical ensemble. The system exhibits two types of interactions: a particle-particle and a particle-porous. In the particle-particle interaction a two lenght scale effective potential with repulsive shoulder at $r/\sigma_{particle} \approx 1$ *and very small attractive part around* $r\sigma_p \approx 3.8$ *is used and the particle-porous interaction is giben by a Weeks-Chandler-Andersen (WCA) potential. In the second approach employs a two-dimensional lattice model defined on a triangular lattice in the grand-canonical ensemble. This model has nearest neighbor interactions given by short-range and hydrogen-bonds energies. Using molecular dynamics simulation, we analyse the influence of the random porous media in the structure of the system through the radial distribution function and the changes in the pressure-temperature phase diagram. In the Monte Carlo simulation we analyse density-chemical potential phase diagram and the number of hydrogen bonds per site.*