Bulk water anomalies and bubble nucleation at negative pressure

A talk by Chantal Valeriani
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Even though water is the most relevant molecule existing in Nature, its anomalous behaviour and properties still lack of a satisfactory understanding. The aim of my talk will be to present our results on determining anomalous properties of bulk water at extreme conditions, and on unravelling the mechanism of bubble nucleation at negative pressure.

Modelling water by means of the TIP4P/2005 interaction potential, we use computer simulations to study properties of bulk water at extreme conditions, i.e. at negative pressure and supercooled. In this region, we find several anomalies: maxima in the adiabatic compressibility, non-monotonic density dependence of the sound velocity and departure from a standard extrapolation of the equation of state. To try to determine the phase diagram of metastable water, we numerically calculate the line of density maxima, the spinodal and the Widom line at negative pressure.

Next, to quantify the mechanism of bubble nucleation from water at negative pressure, we study water at state points both above and below the spinodal line. To compute the nucleation rate and unravel the nucleation mechanism, we use the Mean First Passage Time whereas to estimate the free-energy barrier we use the Umbrella Sampling technique. In both cases, the local order parameter adopted is the volume of the largest bubble.

In the last part of my talk I will present our novel approach to compute the free-energy of solids using both Einstein crystal or Einstein molecules methodologies by means of Molecular Dynamics packages such as GROMACS or LAMMPS.