UNIVERSITÉ DU LUXEMBOURG

Seminar

Thursday, 1st July 2010 at 10:00

Bâtiment des Sciences

Room BS 1.04

Prof. Carlos Vega de las Heras
Universidad Complutense de Madrid

will speak about

" Successes and failures in the description of water when simulating simple models"

Phase diagrams can be evaluated by using computer simulations. For water we have calculated the phase diagram using a number of different empirical potentials: namely TIP3P, TIP4P, TIP5P and SPC/E models. Only the TIP4P model provides a qualitatively correct description of the phase diagram of water and the parameters can be modified slightly to yield an improved water potential : TIP4P/2005. TIP4P/2005 provides a good description of the vapour-liquid equilibria, surface tension, ice properties, maximum in density, structure, equation of state at high pressures, diffusion coefficient, and viscosity. The model is good enough to allow us to explore new physical phenomena for which the experimental results are limited or unavailable, for instance: the existence of a quasi-liquid layer on the free surface of ice , the existence of a liquid-liquid transition in super-cooled water, and the possible appearance of plastic crystal phases in the phase diagram of water. However TIP4P/2005 (as well as other non-polarizable models) fails in the description of the vapour, the dielectric constants of water and ices, and in the evaluation of the heat capacities. The reasons of these failures and the possible solutions will be discussed.