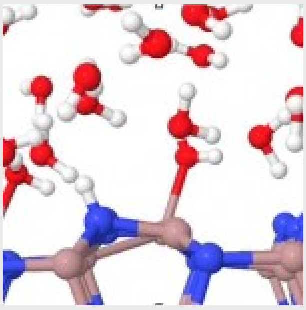
First Principles Understanding of Liquid Water and its Anomalies



Title: First Principles Understanding of Liquid Water and its Anomalies
When: Tuesday, 22 December (2015), 12:00h
Place: Departamento de Física de la Materia Condensada, Facultad Ciencias, Module 3, Seminar Room (5th Floor).
Speaker: Marivi Fernandez-Serra, Physics & Astronomy department, Stony Brook University, New York, USA.

Surprising as it might seem, the understanding of the structure of liquid water is still an open subject, one that has kept theorists and experimentalists busy for the last 50 years. One of the reasons for this is the fact that water is a liquid with a large number of thermodynamical anomalies, and no single theoretical model is capable of explaining them all, or of reproducing all experimental measurements conducted to probe its structure. Advanced computational modeling needs to be developed to simulate the structure and dynamics of liquid water. In this talk, I will show how recent advances within the framework of density functional theory have allowed us to to understand the physics behind some of the anomalies of water.   Our research indicates that the structure and dynamics of liquid water are not so different from its solid phase. In particular, I will show that the hydrogen bond network of water supports propagating optical phonon-like modes.
We argue that on subpicosecond time scales these modes propagate through water's hydrogen bond network over distances of up to two nanometers. In the long wavelength limit these optical modes exhibit longitudinal-transverse splitting, indicating the presence of coherent long range dipole-dipole interactions, as in ice. Our results indicate the dynamics of liquid water have more similarities to ice than previously thought.
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