Appunti di Fisica '18
&
Dottorato di Ricerca in Fisica

4 maggio ore 15:00
Sala seminari, CNR-IPCF

Navigating at Will on the Water Phase Diagram

A. Marco Saitta
(Sorbonne Université, Paris, France)

Despite the simplicity of its molecular unit, water is a challenging system because of its uniquely rich polymorphism and predicted but yet unconfirmed features. Introducing a novel space of generalized coordinates that capture changes in the topology of the interatomic network, we are able to systematically track transitions among liquid, amorphous, and crystalline forms throughout the whole phase diagram of water, including the nucleation of crystals above and below the melting point. Our approach, based on molecular dynamics and enhanced sampling or free energy calculation techniques, is not specific to water and could be applied to very different structural phase transitions, paving the way towards the prediction of kinetic routes connecting polymorphic structures in a range of materials.

http://sites.google.com/site/AppuntiDiFisicaMessina/