

Appunti di Fisica '25

30 Gennaio ore 15:00

Sala seminari, CNR-IPCF

Quantum effects, charge transfer, and electric fields: what matters in water

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What is water? How should we imagine the compound at the basis of life as we know it? In this brief journey, we will try to give an approximate answer to this apparently innocent question.

Owing to the impressive growth of computational power and of the development of novel computational techniques, including data-driven approaches, nowadays it is possible to simulate the behavior of matter with unprecedented reliability. In this talk, I will show how modern path integral ab initio molecular dynamics (PI-AIMD) simulations can shed light on the behavior of protons in water fully including the quantum nature of electrons and nuclei. Besides, I will also show how modern Deep Learning techniques can be exploited in conjunction with classical nuclei AIMD and fully quantum PI-AIMD data to simulate the behavior of liquid water with unprecedented accuracy.

Besides, I will show how electric fields can be tailored to generate a genuine physical response in aqueous systems. In particular, I will present how electric fields can be tuned to induce the electrofreezing phenomenon in bulk water toward a novel exotic phase of water. These field-induced structural and dynamical changes produce important variations of the topology of the H-bond network with crucial impacts in technological apparatus aimed at producing green hydrogen. Finally, if time allows, I will conclude the talk by presenting a novel experimental technique we developed that allows for measuring nuclear and electronic quantum effects in water.