

University of Pavia

Ph.D. School in Electronics, Computer Science and Electrical Engineering
Ph.D. School in Microelectronics

A novel g -sensitive detector apparatus for eV neutron spectroscopy applied to hydrogen bonded systems

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Zoom platform

(<https://us02web.zoom.us/j/85198623155?pwd=emxKc2s0WmtqbU92dmJyNTUxTUx5QT09>)

Abstract: A novel γ -sensitive detector apparatus, named γ DA, and acquisition methodology are developed for eV neutron spectroscopy applied to the characterization of hydrogen-bonded systems. The γ DA is thought to operate on the VESUVIO spectrometer at the ISIS pulsed neutron source and will broaden the capability of neutron scattering at the eV energies in a regime where the nuclear dynamics is probed. Several tests were performed and modelled within the FLUKA environment on a polyethylene sample, used as a neutron spectroscopy standard, in order to find the best experimental configuration. Then the nuclear dynamics of biphenyl, used as a model compound to emulate the lignin decomposition in monocyclic hydrocarbons in the biofuel-production research, was measured with a detection count-rate increase of five times and a signal-background ratio improvement of 50%. The biphenyl dynamics was also simulated with first principles calculations performed within the Quantum Espresso environment and compared with the experimental results accessed by neutron scattering techniques. The simulations allowed to determine the reason why structures with a considerable number of internal vibrations show an isotropic dynamics, *i.e.*, same kinetic energy in all the Cartesian directions as a consequence of the Central Limit Theorem applied to the nuclear dynamics. The γ DA was finally used to demonstrate the unusual stability of ice II. In fact, ice II is the only hydrogen ordered phase that does not have any disordered counterpart and it is stable up to high temperatures. The stability of the phase is motivated by the very low kinetic energy of hydrogens, probed by eV neutron scattering, and by the high displacement, probed by quasi elastic neutron scattering. The hydrogen displacement brings an additional factor to the entropy, a dynamic disorder that makes, together with the low energy, the ice II very stable. Hence ice II is ordered by the disorder, a wonderful joke of Nature.

Organizer

Prof. Lodovico Ratti

Ph.D. Coordinators

Proff. Cristiani and Malcovati

The seminar will take place in English
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