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Neutron-driven exploration of the ice phase diagram

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Water and all its ice forms play a central role in everyday life and science and, as a consequence, the scientific community strives to deepen the knowledge about the polymorphism of ice. Beside this, the investigation of the phase diagram of the solid mixture of water and molecular hydrogen at high pressure has been particularly prolific and associated with exciting discoveries. Several solid stoichiometric and non-stoichiometric phases of the mixture have been characterized in the latest years, some of which, being metastable at ambient pressure and low temperature (77 K), can be recovered and handled in the laboratory. Among these, the so-called C_0 phase led to the discovery, by out-diffusion of hydrogen molecules at about 130 K, of a metastable phase of ice, named afterwards ice XVII. Surprisingly, this low-density solid is highly porous, and presents accessible spiraling channels where hydrogen molecules can be hosted in an essentially one-dimensional geometry. Moreover, by heating above 130 K, ice XVII transforms to metastable ice Ic, having an unprecedented structural purity. In this talk we show how neutron scattering has played an essential role to characterize both the structure and the dynamics of these two elusive forms of ice by reporting accurate studies of their crystal lattice and density of phonon states (DOPSs), as well as the quantum motion of confined H_2 molecules in the ice XVII framework.

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