Contribution ID: **155** Type: **PICO talk**

Quantum dynamics of H2 molecules confined in ice XVII

Tuesday, January 9, 2018 12:35 PM (1h 30m)

Ice XVII is a newly discovered solid form of pure water, which is metastable at ambient pressure if maintained below 130 K. It is obtained from the so-called C0-phase of the H2-H2O binary compound, quenched at a temperature T=77 K, after letting the hydrogen molecules diffuse out of the crystal [1]. It is intrinsically porous and can absorb again molecular hydrogen and release it repetitively, showing a larger or smaller hysteresis depending on the temperature. By means of neutron diffraction, we have recently determined the structure of ice XVII, (hexagonal, with space group P6122) [2]. It presents accessible spiraling channels, where hydrogen molecules have been located during the production and where other molecules (belonging to hydrogen or another gas) can be absorbed again, confined in an essentially one dimensional geometry [2]. This is the second form of metastable ice experimentally obtained by removing weakly-interacting guests (the first being ice XVI, obtained from a neon clathrate [3]), but many low density ice structures have been theoretically studied and found to be possibly stable [4,5]. We present here the results of a new high-resolution inelastic neutron scattering experiment on ice XVII, containing molecular hydrogen with different ortho/para ratio, and with molecular dynamic results. We have unequivocally assigned the measured spectral bands to rotational and center-of-mass translational transitions of either para- or ortho-H2. Reported data demonstrate that H2 molecules rotate almost freely in these nanometric channels, though showing larger perturbation than in clathrate hydrates, and perform a translational motion exhibiting two low frequency excitations. The comparison between the measured spectra and the MD calculations supports the identification of the lowest frequency band as the vibration along the channel direction, while the higher mode corresponds to the motion across the spiral channel. These measurements clearly enable to portray a picture of the confined motions of a hydrophobic guest in this novel inclusion compound [6].

References

[1] L. del Rosso, M. Celli, L. Ulivi, Nat. Commun. 7, 13394 (2016).
[2] L. del Rosso et al., J. Phys. Chem. C 120, 26955 (2016).
[3] A. Falenty, T. C. Hansen, W. F. Kuhs, Nature 516, 231 (2014).
[4] Y. Huang, et al. Science Adv., 2, e1501010 (2016).
[5] Y. Huang, et al. Chem. Phys. Lett. 671, 186 (2017).
[6] L. Ulivi, M. Celli, D. Colognesi, L. del Rosso, S. Rudić, N. English, and C. J. Burnham, Phys. Rev. Material, to be published, arXiv:1706.09350, (2017).

Significance statement

Ice XVII has a unique porous structure. This experimental study of the quantum dynamics of H2 molecules, confined in ice XVII nanometric one-dimensional channels, opens new perspectives for both the modelling of the solid water-hydrogen mixture and for understanding quantum one-dimensional diffusion.

Primary author: Dr ULIVI, Lorenzo (IFAC-CNR)

Co-authors: Dr BURNHAM, Christian J. (School of Chemical and Bioprocess Engineering, University College Dublin, Ireland); Dr COLOGNESI, Daniele (CNR-IFAC); Dr DEL ROSSO, Leonardo (CNR-ISC); Dr CELLI, Milva (CNR-IFAC); Prof. ENGLISH, Niall (University College Dublin, Chemical Engineering); Dr RUDIĆ, Svemir (ISIS Facility, STFC Rutherford Appleton Laboratory)

Presenter: Dr ULIVI, Lorenzo (IFAC-CNR)

Session Classification: Poster & Lunch