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Formation of a Quasi 2D-layer of Protons in Hydroxides at High Pressure ROMAIN DUPUIS, Donostia International Physics Center, JORGE DOLADO, Tecnalia, JOSE SURGA, Intevp, MAGALI BENOIT, Cemes, ANDRES AYUELA, Cfm — In this work, we found that a remarkable quasi 2D-layer of protons is formed in hydroxides at high pressure[1]. Among numerous fields, hydroxides are used in chemistry, in the industry (glass, cements) and in geosciences (water retainer, mantle crust). We investigated the dynamical properties of protons considering key nuclear quantum effects. For that, we used the Path Integral Molecular Dynamics method that has become a reference[2, 3]. An archetype system ($\text{Ca}(\text{OH})_2$) was considered. We found that a 2D-layer of protons is formed at high pressure. A new mechanism, consisting of quantum rotations of protons, controls the diffusion of protons in hydroxides. [1](Submitted to PRL) R. Dupuis, J. Dolado, J. Sarga, M. Benoit, A. Ayuela [2]O. Marsalek, C. Pei-Yang, R. Dupuis, M. Benoit, M. Méheut, Z. Bacic and M. Tuckerman, *J. of Chemical Theory and Computation*, v. 10, no. 4, pp. 1440–1453, 2014. [3]J. Cao and G. A. Voth, *J. Chem. Phys.*, v. 100, no. 7, pp. 5106–5117, 1994.

Romain DUPUIS
Donostia International Physics Center

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