

Formation of a Quasi 2D-layer of Protons in Hydroxides at High Pressure

Romain Dupuis¹, Jorge Dolado², Jose Surga³, Magali Benoit⁴ and Andrés Ayuela¹

¹DIPC, paseo manuel de Lardizabal, 4, 20018, San Sebastian

²Tecnalia,

³Intevp, Parque Científico y Tecnológico de Bizkaia

⁴CEMES, 29 rue Jeanne Marvig, 31000 Toulouse

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).

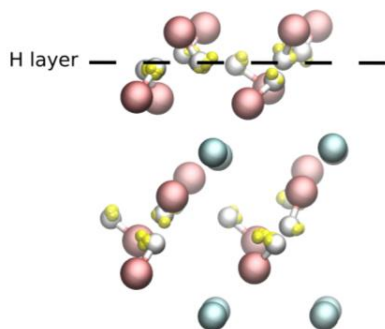


Figure 1. snapshot of the simulation showing the formation of the 2D-layer.

We investigated the dynamical properties of protons. For that, we used the Path Integral Molecular Dynamics method that has become a reference to consider the nuclear quantum effects^[2,3]. We found that a new mechanism, consisting of rotations of protons, tempers the diffusion of protons in hydroxides at high pressure.

[1] R. Dupuis, J. Dolado, J. Surga, M. Benoit, A. Ayuela, *submitted to Scientific Reports*.

[2] O. Marsalek, C. Pei-Yang, R. Dupuis, M. Benoit, M. Méheut, Z. Bacic and M. Tuckerman, *J. of Chemical Theory and Computation*, **10**, 1440-1453, 2014.

[3] J. Cao and G.A. Voth, *J. Chem. Phys.*, **100**, 5106-5117, 1994.