

## **Confinement of a water fluid film during crystallisation in a porous material**

A. Barthes<sup>a\*</sup>, M. Pérez-Rodríguez<sup>a</sup>, T. Bernet<sup>b</sup>, M. M. Piñeiro<sup>c</sup>, M. M. Conde<sup>d</sup>, D. Grégoire<sup>a,e</sup>, C. Miqueu<sup>a</sup>

<sup>a</sup>Université de Pau et de Pays de l'Adour, E2S UPPA, CNRS, LFCR, Anglet, France

<sup>b</sup>Department of Chemical Engineering, Imperial College London, UK

<sup>c</sup>Universidad de Vigo, Vigo, Spain

<sup>d</sup>Universidad Politécnica de Madrid, ETSII, IQI, 28006, Madrid, Spain

<sup>e</sup>Institut Universitaire de France, Paris, France

\*corresponding author: abarthes@univ-pau.fr

### **Abstract:**

Water confined in porous materials has attracted great attention due to its large number of applications such as the conservation of porous building materials in civil engineering. Crystallization of water in porous media involves extremely high pressures able to produce the deformation of the porous matrix. When crystallization occurs in a pore, the interactions between the crystal and the skeleton have led to the concept of “crystallization pressure”<sup>1</sup>. It has been supposed that the interaction should be mediated by the presence of a thin water fluid film (a few nanometer thick) located in between them.

This study aims to describe the thin water film occurring between the ice crystal and the solid surface of a porous material during crystallization and to compute the pressure of this inhomogeneous film. A molecular non-local Density Functional Theory (NLDT)<sup>2</sup> coupled with the Statistical Associative Fluid Theory for potential of variable range (SAFT-VR)<sup>3</sup> has been developed and employed to obtain the equilibrium distribution of water molecules confined into this slit-like nanopore consisting of the wall of ice on one side and a graphitic surface on the other side. Several configurations are explored by changing both the thermodynamic conditions and the water film width.

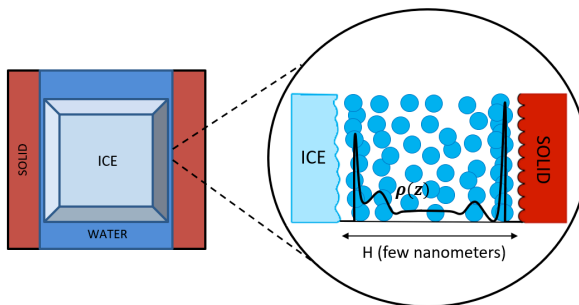


Fig. 1. Ice crystal confined between two solid surfaces of a slit pore. Thin water film between a wall of ice and a graphitic surface with a schematic representation of the asymmetric water density profile  $\rho(z)$  obtained at equilibrium with NLDT-SAFT-VR coupling.

**Acknowledgements:** This work is financed by the Investissement d'Avenir French programme (ANR-16-IDEX-0002) under the framework of the E2S UPPA hub Newpores.

---

<sup>1</sup> Scherer, G.W. (2004). *Cement Concrete Res.* **34** (9), 1613-1624.

<sup>2</sup> Evans, R. (1979). *Advances in Physics* **28**, 143.

<sup>3</sup> Chapman, W.G. and Gubbins, K.E (1989). *Fluid Phase Equilibria.* **52**, 31-38.