

## Hydrogen bond dynamics in amorphous carbonate precursors

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Amorphous calcium carbonate (ACC), the precursor to a wide variety of biominerals, has a highly hydrated and disordered structure [1]. An important role of water in their stability has been suggested by modeling studies [2], yet still there is a lack of experimental studies addressing the water structure and dynamics. Here, we investigate a series of pure and Mg-bearing ACC, using techniques such as TGA, FTIR and Incoherent Inelastic Neutron Scattering (IINS) experiments. This last technique is aimed at obtaining dynamical information on the strength of the hydrogen bond network around the hydrated cations. Ab-initio calculations and classical MD simulations were used to analyze the IINS spectra.

TGA and FTIR analysis reveal that different types of water are present in the amorphous structure. In addition, IINS results indicate the presence of a strong H-bond network, whose stability, however, is independent on the degree of Mg<sup>2+</sup> bearing. These results imply the existence of confined water in structural ‘pockets’ in ACC, resulted presumably from the aggregation processes during densification of the Ca-Mg-CO<sub>3</sub> structure, pointing to a secondary role of water in the amorphous structure.

[1] Addadi, L. et al. (2003) *Adv. Matter* **15**, 959–970. [2] Raiteri, P. & Gale, J. D. (2010) *J. Am. Chem. Soc.* **132**, 17623–17634.