The role of polyaspartic acid on the kinetic persistance of amorphous calcium carbonate

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Amorphous calcium carbonate (ACC) is a metastable precursor phase of calcium carbonate commonly found in biominerals [1]. The presence of organic molecules (e.g., aminoacids such as polyaspartic acid –pAsp– has been found to be a key on the kinetic persistence of ACC strongly influencing its crystallization kinetics [2]. Despite the important insights provided by earlier studies, the specific mechanisms of stabilization and their link to structural dynamics and crystallization kinetics are poorly understood.

Various authors have suggested that the water structure and hydrogen bonding are important factors enhancing the kinetic stability of ACC [3]. Here, we investigate the dynamic properties of water present in pure ACC compared with dopped ACC with pAsp. With that aim, pure ACC and pAspbearing ACC have been analyzing using thermogravimetric analysis (TGA) and Fourier transform infrared spectroscopy (FTIR) combined with the Incoherent Inelastic Neutron Scattering (IINS) technique, which provides information on the strength of the hydrogen bond network and it is highly sensitive to intermolecular interactions of water molecules.

Our results suggest that, similarly as observed for Mg^{2+} [3], the presence of pAsp in ACC could enhance the persistence of water within the nucleated particles, which facilitates the formation the ACC due to the formation of a strong hydrogen bonding network delaying crystallization of anhydrous calcite.

[1] Addadi et al., 2003. Adv. Matter 15, 959-970.

- [2] Zou et al., 2017. Small 13, 13, 1-11.
- [3] Koishi et al. 2018, J. Phys. Chem. C, 122, 16983-16991.