Modelling calcium phosphate pre-nucleation events

RAFFAELLA DEMICHELIS,[1*] NATALYA GARCIA,[1] PAOLO RAITERI,[1] JULIAN D. GALE,[1] RICCARDO INNOCENTI MALINI,[2] COLIN L. FREEMAN,[2] JOHN H. HARDING[2]

[1]Curtin Institute for Computation, The Institute for Geoscience Research, and Department of Chemistry, Curtin University, Perth, WA, Australia, raffaella.demichelis@curtin.edu.au (* presenting author)

[2]Department of Materials Science and Engineering, University of Sheffield, Sheffield, United Kingdom

A model[1] able to capture the dynamics and the thermodynamics of processes at the calcium phosphate-water interface has been developed. This was obtained through fitting to multiple calcium phosphate minerals, the water structure around the different ions and the thermodynamics of the ions in solution. The aim is to explore the possibility of nucleation pathways alternative to those proposed by the classical nucleation theory.

The atomic details regarding the free ions in solution (e.g. Figure 1) and the first association events, i.e. the formation of ion pairs and of small clusters, are discussed and compared to the available experimental data[2], to existing theoretical estimates [3] and to results obtained for other minerals[4,5].

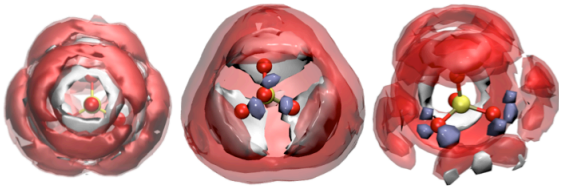

Figure 1. From left to right: Representation of the water structure around PO_4^{3-}, HPO_4^{2-}, and $H_2PO_4^-$. Isosurfaces: red for O of water, white for H of water, purple for H of phosphate. Atoms: red for O and yellow for P.

[1] Demichelis et al. *in preparation*
[2] Busenberg & Plummer. *Geochimica et Cosmochimica Acta* **1989**, *53*, 1189
[3] Marcus. *Biophysical Chemistry* **1994** *51*, 111
[4] Pegado et al. *Phys. Chem. Chem. Phys.* **2012**, *14*, 10248
[5] Raiteri et al. *J. Phys. Chem. C* **2015**, *119*, 24447