Modelling calcium phosphate pre-nucleation events

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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 PO₄³⁻, HPO₄²⁻, and H₂PO₄⁻. 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