Interaction of stable aggregates drives the precipitation of calcium phosphate in supersaturated solutions

Supplementary information

R. Innocenti Malini¹*, C. Freeman², J. H. Harding²

¹ Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Biomimetic Membranes and Textiles, St. Gallen 9014, Switzerland
² Department of Materials Science and Engineering, University of Sheffield, Mappin Street, Sheffield S1 3JD, U.K.

*Corresponding author:
Riccardo.innocentimalini@empa.ch
Figure S1. Snapshots of nanoparticles from different simulations. a, b and c are described in the figure. In the image, the Ca$^{2+}$ is coloured in cyan, phosphorous in green, oxygen in red and hydrogen in white.

Figure S2. Tetrahedral order parameter of water, $q$, as a function of the distance from the centre of mass of CO$_3^{2-}$ (blue) and HPO$_4^{2-}$ (orange). The tetrahedral order parameter is defined as:

$$q = 1 - \frac{3}{8} \sum_{j=1}^{3} \sum_{k=j+1}^{4} \left( \cos \varphi_{jk} + \frac{1}{3} \right)^2$$

where $\varphi_{jk}$ is the angle between the vectors from an oxygen atom of a water molecule to the oxygen atoms of its two nearest neighbours.
Force field input file used in LAMMPS

variable P equal 1
variable O9 equal 2
variable O8 equal 3
variable H8 equal 4
variable OW equal 5
variable HW equal 6
variable CA equal 7

mass ${P} 30.974
mass ${O9} 16.000
mass ${O8} 16.000
mass ${H8} 1.000
mass ${OW} 15.999
mass ${HW} 1.001
mass ${CA} 40.078

bond_style hybrid harmonic
#@ P - O9
bond_coeff 1 harmonic 21.570600 1.52000
#@ P - O8
bond_coeff 2 harmonic 12.117050 1.60000
#@ O8 - H8
bond_coeff 3 harmonic 21.576300 0.98000
#@ OW - HW
bond_coeff 4 harmonic 22.965000 1.01200

angle_style hybrid harmonic class2
#@ O9 - P - O9
angle_coeff 1 class2 109.50000 5.9375000 0.0000000
angle_coeff 1 class2 bb 1.61990 1.5200000 1.5200000
angle_coeff 1 class2 ba 0.00000 1.5200000 1.5200000
#@ O8 - P - O9
angle_coeff 2 class2 109.50000 2.2033000 0.0000000
angle_coeff 2 class2 bb 2.91010 1.5200000 1.6000000
angle_coeff 2 class2 ba 0.00000 1.5200000 1.5200000
#@ H8 - O8 - P
angle_coeff 3 harmonic 1.45275 111.40000
#@ HW - OW - HW
angle_coeff 4 harmonic 1.645680 113.24000

dihedral_style hybrid charmm
#@ H8 - O8 - P - O9
dihedral_coeff 1 charmm 0.042272 3 180 0.0

pair_coeff ${OW}  ${OW}  lj/cut  0.006738  3.165572

pair_modify tail yes

pair_coeff ${O8}  ${O8}  buck/mdf  12534.455000  0.202  0.
pair_coeff ${O9}  ${O8}  buck/mdf  12534.455000  0.202  0.
pair_coeff ${O9}  ${O9}  buck/mdf  12534.455000  0.202  0.
pair_coeff ${O8}  ${H8}  lennard/mdf  54.  0.
pair_coeff ${O9}  ${H8}  lennard/mdf  54.  0.

pair_coeff ${O8}  ${OW}  buck/mdf  19534.455133  0.2151  0.
pair_coeff ${O9}  ${OW}  buck/mdf  19534.455133  0.2426  0.

pair_coeff ${O8}  ${CA}  buck/mdf  2010.878     0.276289   0.
pair_coeff ${O9}  ${CA}  buck/mdf  2590.878     0.276289   0.

pair_coeff ${P}    ${P}                       coul/long
pair_coeff ${P}    ${O9}                       coul/long
pair_coeff ${P}    ${O8}                       coul/long
pair_coeff ${P}    ${H8}                       coul/long
pair_coeff ${P}    ${OW}                       coul/long
pair_coeff ${P}    ${HW}                       coul/long
pair_coeff ${O9}   ${O9}                       coul/long
pair_coeff ${O9}   ${O8}                       coul/long
pair_coeff ${O9}   ${H8}                       coul/long
pair_coeff ${O9}   ${OW}                       coul/long
pair_coeff ${O9}   ${HW}                       coul/long
pair_coeff ${O8}   ${O8}                       coul/long
pair_coeff ${O8}   ${H8}                       coul/long
pair_coeff ${O8}   ${OW}                       coul/long
pair_coeff ${O8}   ${HW}                       coul/long
pair_coeff ${H8}   ${H8}                       coul/long
pair_coeff ${H8}   ${OW}                       coul/long
pair_coeff ${H8}   ${HW}                       coul/long
pair_coeff ${OW}   ${OW}                       coul/long
pair_coeff ${OW}   ${HW}                       coul/long
pair_coeff ${HW}   ${HW}                       coul/long
pair_coeff ${P}    ${CA}                       coul/long
pair_coeff ${O9}   ${CA}                       coul/long
pair_coeff ${O8}   ${CA}                       coul/long
pair_coeff  ${H8}  ${CA}                      coul/long
pair_coeff  ${CA}  ${CA}                      coul/long
pair_coeff  ${OW}  ${CA}                      coul/long
pair_coeff  ${HW}  ${CA}                      coul/long