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An Alternative Reaction Scheme for Calcium Phosphate Nucleation on Silica Glass Ceramics: Molecular Dynamics Simulations[1]
BERNARD DELLEY, RENE WINDIKS, Paul Scherrer Institut, Switzerland —
The silica mineral α-wollastonite exposed to physiological aqueous solutions induces the nucleation of calcium phosphate (CaP) on its surface. The nucleation is the initial step of the formation of biological-like CaP layers which finally provide an ideal environment for a strong bonding to biological tissues and mature bone. However,the mechanism of nucleation and the molecular structure of the first inorganic precipitates is still under investigation. We have performed density functional molecular dynamics simulations on model systems and propose a nucleophilic substitution reaction type which includes the formation of covalent Si–O–P linkages. Initially, oxygen atoms of phosphate ions attach to silicon atoms of the solvated silica species at the surface of the mineral. Subsequently, a Si–O bond is formed and the silicon atom has a penta-oxo coordination. Finally, another Si–O bond of the pentacoordinated silicon is broken.The calculated change of the Helmholtz free energy is negative. That is, the reaction ends with CaP strongly bonded to the mineral. The reaction barriers along this pathway remain fairly low, as the pentacoordinated Si is part of a metastable intermediate state.

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Bernard Delley
Paul Scherrer Institut Switzerland

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