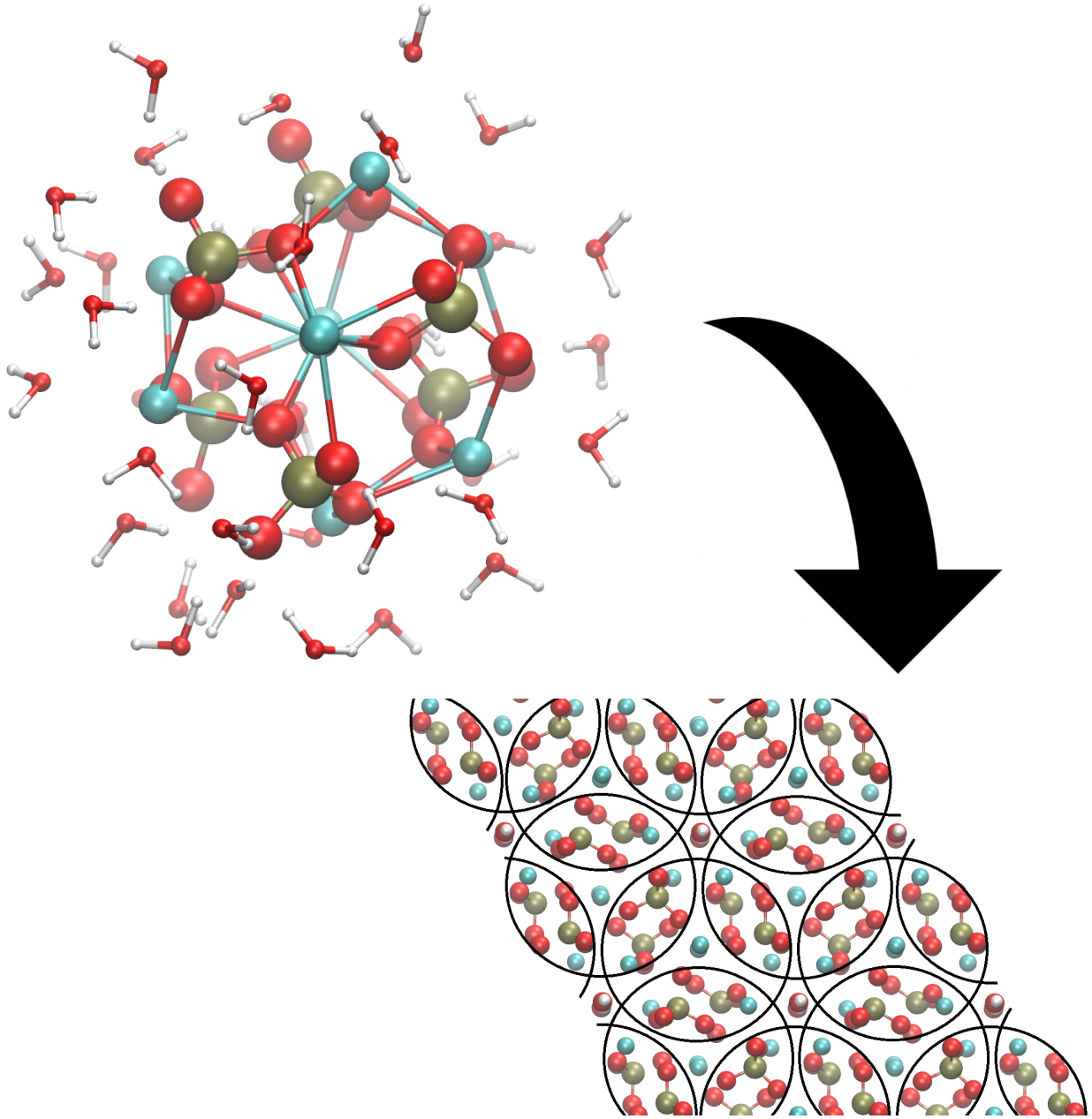

Bones and teeth are composite materials made of an organic component, a helical protein named collagen and an inorganic component, calcium phosphate. Although calcium phosphate is found in nature as a variety of polymorphs, the most stable one is hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$, shown projected on the xy plane in the image at the bottom right). The spherical cluster in the image at the top left is a Posner's cluster. The Posner's cluster is the building block of several calcium phosphates including hydroxyapatite. It is roughly spherical with a diameter of ≈ 1 nm, and chemical formula $Ca_9(PO_4)_6$. This cluster was first discovered by two researchers, Betts and Posner, in the seventies, during an X-ray diffraction experiment on amorphous calcium phosphate; it has been later detected in the body fluids and therefore it is currently object of investigations targeted to discover its role in calcium phosphate formation.

Our research consisted in simulating the behaviour of calcium and phosphate ions in water at body temperature using classical Molecular Dynamics with the aid of a supercomputing facility. We observed the aggregation of the ions to form large clusters; a thorough examination of the latter showed the presence of several Posner's clusters within them. Afterwards, we simulated a series of solutions with different composition: a change in pH was achieved tuning the ratio among the phosphate species (HPO_4^{2-}, $H_2PO_4^-$ and PO_4^{3-}); in physiological conditions (pH $\approx$ 7.4) the phosphate ions are mainly present in the protonated form. We also added sodium ions, which are abundant in the body fluids, to see how their presence affects the calcium phosphate aggregation. The Posner's clusters were also detected altering the composition of the initial solution, hence we were able to validate the assumption that these clusters form spontaneously in water and play a fundamental role in calcium phosphate formation in the body fluids.