Computational chemistry as the missing piece in the characterization puzzle of biological mineralization

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Resumen

Solids of biological origin such as hydroxyapatite or calcium oxalates are directly involved in chemistry of “life”: Hydroxyapatite as the main compound of human bones and calcium oxalate as main compound of kidney stones. In this broad study around chemistry of life, materials chemistry and computational chemistry we focus here on Calcium Oxalate and Hydroxyapatite.

We have performed DFT studies on different interfaces and investigated the interaction with a series of bio-organic molecules, and characterized them by calculating vibration frequencies and chemical shifts, which were compared to experimental data.

From the bulk crystal structures of calcium oxalate polymorphs obtained through DFT methods[1, 2, 3] the low index surfaces were build. Since the thermodynamic stability depends on the medium in which the surface is introduced, the calculation of the interaction of the calcium oxalate surface with water, urea, and other small molecules gives us the possibility to understand the change in crystal morphology of the final oxalate crystal in its natural medium. The final aim is the prediction of the shape of the kidney stone in its natural medium.

Another biological mineral that we have studied is hydroxyapatite, being the major mineral component of tooth enamel, dentin and bone in which it is currently associated to biomolecules and various biopolymers. Organic nanosized particles are described as comprising a core surrounded by a crystalline hydrated amorphous layer. In this study the characterization of the surface of hydroxyapatite nanoparticles is essential to better understand their formation, and dissolution mechanisms and interactions existing at the interface between the crystalline and amorphous phases. The purpose of this study is to model a surface(s) of hydroxyapatite and analyze the physicochemical properties using the methods of quantum chemistry (periodic DFT).