Computational investigation of the crystallization of calcium oxalate.

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The formation and growth of calcium oxalate minerals is associated with a variety of biological processes in micro-organisms, plants, fungi, and animals, [1] including some pathological mechanisms in humans such as kidney stones and breast cancer.[2] [3] In the environment, they represent the most common family of organic minerals occurring in sediments and hydrothermal veins [4]. However, little research has been devoted so far to understand their nucleation, growth, and properties.

As for many minerals, a variety of stable and metastable anhydrous and hydrated crystalline structures have been observed, [4] though their details are yet to be fully explored. Similarly, the dynamics of their nucleation and of their interaction with aqueous solutions is not yet fully understood.

In the present study we apply computer simulation techniques to investigate several steps relating to the formation of these minerals. This presentation will focus on the structural features of many species that can nucleate and phases that can grow from aqueous solution, and on the possible transformation mechanisms from one to another.

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