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Crystallographic properties of the calcium phosphate mineral, brushite, by means of First Principles calculations

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ABSTRACT

A crystalline form of hydrated calcium phosphate, brushite ($CaHPO_4 \cdot 2H_2O$), has been studied by means of total energy First Principles calculations based on the Density Functional Theory (DFT) approximation. The experimental crystal lattice parameters of this mineral have been reproduced with good agreement. The powder X-ray diffraction pattern simulated from the calculated crystal structure is similar to the experimental one. The intermolecular interactions within the crystal, electrostatic and hydrogen bond interactions, have been reproduced. The calculated crystal structure reproduces the atomic distribution along the (010) surface observed by high resolution scanning force microscope (SFM). The optimized crystal structure describes the different interatomic interactions along the [101], [201], and [001] directions on the (010) plane. Quantum-mechanical calculations of the energy of these surfaces confirm the experimental behavior, justifying the different crystal growth rates of these directions found experimentally.