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First principles study of biomineral hydroxyapatite ALEXANDER SLEPKO — Hydroxyapatite (HA) [$Ca_{10}(PO_4)_6(OH)_2$] is one of the most abundant materials in mammal bone. It crystallizes within the spaces between the tropocollagen chains and strengthens the bone tissue. The mineral content of human bone increases with age reaching a maximum value from which it starts to decrease leading to diseases such as osteomalacia. Therefore, an emergent application of this study is bone repair and the production of synthetic bone. Despite its importance, little is known about the growth of HA crystallites in bones. Nor is it well understood how the HA attaches to protein chains and interacts with the surrounding aqueous solution. Using density functional theory (DFT) we calculate the theoretical ground state structure, electronic and vibration properties of hexagonal HA. We find several low energy structures and analyze the energy barriers for spontaneous phase transitions. We calculate the phonon density of states and study the surface energetics for different orientations. We identify the surfaces with highest reactivity using the frontier orbital approach and analyze interactions between these surfaces and water molecules/amino acids.

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