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Bone mineral: first principles study of carbonate substitutions in hydroxyapatite[1] ROOPE ASTALA, MALCOLM J. STOTT, Department of Physics, Queen's University, Canada — Mineral components of bone and teeth are hydroxyapatite at varying crystallinities and impurity concentrations, with carbon as a CO_3^{-2} ion being the most abundant. The impurities influence the biological properties of bone and a study of their electronic and structural nature will contribute to a full understanding of the biological aspects. We perform electron density functional theory calculations to investigate CO_3^{-2} on different sites in periodic hydroxyapatite lattice, as well as various charge compensation mechanisms. These include substitutions on OH^- (A-site) and PO_4^{-3} (B-site), and compensation by V_{OH} or V_{Ca}. Defect clustering and effects of impurity concentration are studied. Substitutions of two CO_3^{-2} for two PO_4^{-3}, compensated by a V_{Ca}, were found to be the most favored energetically. The a lattice parameter increases for A-site substitutions, while for the B-site it typically decreases. The implications on the material properties are discussed.

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