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First-principles Study of the Removal of Boron by Co-precipitation with Hydroxyapatite Using Dolomite as a Starting Material CHENYANG LI, LAZARO CALDERIN, Pennsylvania State University, KEIKO SASAKI, Kyushu University, ISMAILA DABO, Pennsylvania State University, PENNSYLVANIA STATE UNIVERSITY COLLABORATION, KYUSHU UNIVERSITY COLLABORATION — Boron is a toxic chemical in drinking water and a major health concern worldwide. One method to reduce boron concentration in water consists of co-precipitating boron with hydrated minerals. Nevertheless, little is known about the chemical mechanisms underlying boron reactions with complex minerals. In this work, we have applied first-principles calculations based on density-functional theory (DFT) to characterize boron-bearing hydroxyapatite (HAp) resulting from co-precipitation with hydrated dolomite. DFT calculations have been performed to interpret X-ray diffraction (XRD) and nuclear magnetic resonance (NMR) experiments and to characterize solid residues after boron removal with a focus on determining the absorption sites of $B(OH)_3$ and $B(OH)_4$ in the formed minerals. The computed results indicate that the absorption takes place at phosphate (PO_4) sites. In addition, changes in the lattice parameters of B-bearing HAp as a function of boron concentration have been calculated and compared with experimental results. Good agreement of the decreasing trend in a-direction and the increasing trend in c-direction has been observed by our calculations. Raman and infrared (IR) spectra have been studied as well to achieve a better understanding the B-HAp structures.

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