

A DFT, X- and W-band EPR and ENDOR Study of Nitrogen-Centered Species in (Nano)Hydroxyapatite

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Abstract

Incorporation of the nitrogen-containing impurities in hydroxyapatite (HAp) powders with the sizes of the crystallites of (20-50) nm was studied using first-principles modeling combined with the multi-frequency (9 and 94 GHz) electron paramagnetic resonance (EPR) methods. It is shown that the observed EPR spectra are undoubtedly due to the presence of the bulk radiation-induced NO₃²⁻ radicals. This conclusion is based on spin-polarized density functional theory calculations of spectroscopic parameters within gauge-including projector augmented wave framework followed by the exact comparison of the simulated EPR and electron-nuclear double resonance spectra with the experimental findings. In addition, a comprehensive analysis of the simulated properties allows us to suggest that the paramagnetic centers preferably occupy PO₄³⁻ sites in the HAp structure. © 2014 Springer-Verlag Wien.

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