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A DFT, X- and W-band EPR and ENDOR study of nitrogen-centered species in (Nano)hydroxyapatite

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Abstract

© Springer-Verlag Wien 2014. 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 NO_3^{2-} 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 PO_4^{3-} sites in the HAp structure.

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