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First-Principles Solid-State Calculations and Pulsed EPR Measurements: a Study of Ionic Substitutions in Hydroxyapatite

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Density functional theory (DFT) calculations are widely used to characterize the electronic structure and magnetic resonance parameters of paramagnetic molecules. Here we address the versatility of plane-wave DFT for studying impurities in solids in combination with pulsed EPR techniques. We focus on hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$ (nano)crystals as a host lattice, since it is very tolerant to many ionic substitutions. We show that the calculation of magnetic resonance parameters in conjunction with EPR/ENDOR experiment can successfully complement first-principles thermodynamic analyses of the impurity localization. Next, we attempt to connect the results of electron spin-lattice relaxation measurements with the calculated phonon properties of the host crystal. Finally, we illustrate the capabilities of the combined experimental-computational approach for studying the interplay of oppositely charged substitutions (Pb^{2+}, Mn^{2+}, CO_2^- and NO_3^{2-} ions) in the structure of hydroxyapatite nanopowders.

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