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Order-disorder effects and self-activated photoluminescence in hydroxyapatite nanoparticles via impurities incorporation

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Hydroxyapatite (HA) is a widely studied material in biomedical areas, due to its properties such as high biocompatibility, bioactivity and controlled biodegradability. (1) In nanomedicine, HA nanoparticles (NPs) have been explored as important tools for the image diagnosis and therapy of diseases such as cancer. (2) Specifically, the diagnostic function of HA NPs can be improved via the inclusion of structural defects during the synthesis or subsequent heat treatment. (3) This study aims to demonstrate the influence of carbon-associated defects on the self-activated photoluminescence of HA. The NPs were synthesized by a simple chemical precipitation followed by heat treatment at 400°C/4h. The long- and short-range order of as-synthesized and heat-treated samples were characterized, evidencing an increase in lattice disorder as a function of impurities concentrations. The Fourier transform infrared (FTIR) spectra were used to estimate the concentrations of the impurities, confirming their incorporation (0.6 wt.% to 10.8 wt.%) and partial elimination after the heat treatment. Thermogravimetric analysis (TGA) evidenced that the main mass loss in the temperature range studied is related to structural water elimination and partial elimination of introduced impurities. Transmission electron microscopy (TEM) analysis revealed that the samples comprise of nanorods with sizes below 40 nm. PL spectroscopy revealed that degree of incorporation of impurities affected the intensity, position, and broadness of the defect-related broadband emission when excited at 405 nm, confirming their impact on PL properties of HA NPs. **Acknowledgments:** Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP), grants nº 2022/14435-8, 2020/14417-4, and CNPq, grant nº 164373/2020-9

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