

# Effect of Zr ions in photoluminescence properties of CCTO obtained by the soft chemical method

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This letter reports on a process to prepare nanostructured  $\text{CuCa}_3\text{Ti}_{0.6}\text{Zr}_{0.4}\text{O}_{12}$  (CCTO) at room temperature with photoluminescence (PL) emission in the visible range. Ultraviolet-visible absorption spectroscopy, photoluminescence<sup>(1)</sup>, and first principles quantum mechanical measurements were performed. The ultrafine  $\text{Ca}_3\text{CuTi}_{0.6}\text{Zr}_{0.4}\text{O}_{12}$  powders calcinated at 300°C and 700 °C for 2 h presents intense visible photoluminescence behavior at room temperature. The increase of temperature and annealing time creates  $\text{TiO}_5$  clusters in the lattice leading to the trapping of electrons and holes. Thus,  $\text{TiO}_5/\text{TiO}_6$  clusters were the main reason for the PL behavior. These results suggest that the temperature modifies the particle's structure, resulting in localized states in an interfacial region between the crystalline and amorphous  $\text{Ca}_3\text{CuTi}_{0.6}\text{Zr}_{0.4}\text{O}_{12}$ .

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[1] Rosana F. Gonçalves, Neftalí L. V. Carreño, Márcia Tsuyama Escote, Kírian Pimenta Lopes, Antoninho Valentini, Edson R. Leite e Elson Longo. Fotoluminescência e Adsorção de  $\text{CO}_2$  en Nanopartículas de  $\text{CaTiO}_3$  Dopadas Com Lantânio. *Quim. Nova*, Vol. 27, No. 6, p. 862-865, 2004.

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