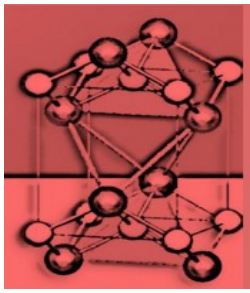

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Structural, electronic and optical properties of TiO_2 nanoparticles and derived sodium titanate nanotubes $Na_2Ti_2O_5.H_2O$ doped with transition metals (Fe, Cu, Ni). A theoretical-experimental study

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This work presents the synthesis, structural characterization, and optical properties of anatase nanoparticles, both pure and doped with transition metals (Fe, Cu, Ni), obtained via modified sol-gel methods [1]. Additionally, it compares these nanoparticles with doped $Na_2Ti_2O_5.H_2O$ titanate nanotubes derived from the precursor nanoparticles. A structural model for onedimensional nanostructures is proposed, based on first principles, which successfully accounts for the complex diffraction patterns observed in the system [2].

The optical properties, particularly the bandgap energies and Urbach tails, were studied to enhance the model describing the absorption edge of the materials. This study aims to understand the impact of doping atoms on the electronic properties and, consequently, the optical behavior of the materials. The main findings indicate that the anatase nanoparticles exhibit no significant changes in bandgap energies. However, a moderate red shift is observed in the indirect bandgap energies of the nanotubes. All doped samples show higher Urbach energies compared to the pristine ones, suggesting the introduction of impurity electronic states within the bandgap. Furthermore, greater optical activation is noted, evidenced by higher Urbach energies in sodium dititanate systems compared to anatase nanoparticles. These observations are consistent with our electronic and optical DFT [3,4] calculations. The phenomena can be interpreted in terms of the hybridization characteristics of the impurity states introduced into the electronic gap.

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