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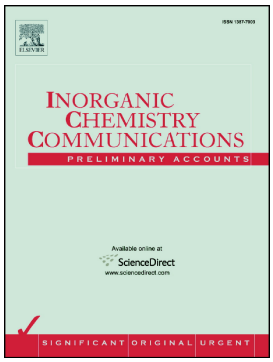

Electronic structure, growth mechanism, and sonophotocatalytic properties of sphere-like self-assembled NiWO4 nanocrystals

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Electronic structure, growth mechanism, and sonophotocatalytic properties of sphere-like self-assembled $NiWO_4$ nanocrystals

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Abstract: In this communications, we report the synthesis of nickel tungstate ($NiWO_4$) nanocrystals by controlled co-precipitation at 95 ºC for 2 h, followed by heat treatment at 600 ºC for 2 h. The structure of the $NiWO_4$ nanocrystals was characterized using X-ray diffraction (XRD) and Rietveld refinement analysis. Field emission-scanning electron microscopy (FE-SEM) was employed to observe the shape, average size and propose a growth mechanism for the synthesized $NiWO_4$ nanocrystals. The optical behavior was investigated by ultraviolet−visible (UV–Vis) spectroscopy and first-principles quantum mechanical calculations based on the density functional theory at the B3LYP level to obtain their electronic band structure and density of states. We investigated the sonophotocatalytic (SPC) properties of the remazol brilliant violet 5R (RBV5R) anionic dye for degradation using a violet light emitting diode of power 10 W. The XRD patterns indicate that the $NiWO_4$ nanocrystals heat-treated at 600 ºC for 2 h have a wolframite-type monoclinic structure. The FE-SEM images showed the presence of irregular sphere-like crystals formed by self-assembly of several $NiWO_4$ nanocrystals. The experimental optical band gap energy ($E_{gap(exp)}$) was found to be 2.77 eV using UV–Vis spectroscopy and theoretical calculations indicate an indirect band gap with E_{gap} 3.91 eV, which the (O 2*p* orbitals) are predominant in the valence band and the (W 5*d* orbitals) in the conduction band and inhomogeneous electronic distribution into the lattice with the electron density map. We demonstrate for the first time that SPC activity can be enhanced after 120 min by approximately 32% for the degradation of the RBV5R anionic dye by using a $NiWO_4$ nanocatalyst.

***Keywords*:** *$NiWO_4$ nanocrystals; Growth mechanism; Optical band gap; Band structure; Sonophotocatalysis*

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