

Influence of the interface STO in the Rhodamine B photodegradation process

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Abstract – Ceramics based on SnO₂-TiO₂ system are important due to catalytic properties yield for ultraviolet radiation (UV). However, formation of SnO₂ nanoislands are reported as factor of influence in the results catalytic. The present paper shows an investigation about catalytic properties of the SnO₂-TiO₂ system with structure type rutile subjected at temperatures in the range 500-1200°C. It were realized simulations of the Sn_xTi_{1-x}O₂ structures by methodology DFT/B3LYP, spatial group P₄₂/mnm using CRYSTAL06 code. It was used to investigation dye Rhodamine B photodegradation, density of states (DOS) and band gap.

In the literature is found papers about nanoisland synthesis methods for some materials^{1,2}. Sn_xTi_{1-x}O₂ solid solution calculations were reported in DFT/B3LYP methodology to investigate alterations in the structure electronic and optical properties³. SnO₂-TiO₂ (x = 0; 0.25; 0.50; 0.75; 1) samples were obtained via Pechini method. Samples were pre-calcined at 450°C for 3h and thereafter calcined at different heat treatment temperature in the range 500-1200°C. XRD results showed that rutile phase is the structure domain in the SnO₂-TiO₂ samples. This difference in the catalytic behavior is due to energy levels, which are modified in relation to average particle size. The efficiency of catalytic process increase because of the formation of Sn_xTi_{1-x}O₂ interface among SnO₂-TiO₂ particles (Figure 1). This process yield formation of SnO₂ particles in the surface of TiO₂ particles bonded for a interface Sn_xTi_{1-x}O₂ (Figure 2a). Difference of decay between STO interface and SnO₂ particle is difficult to note due to similar band gap (Figure 2b). This behavior can be discuss in relation to presence of vacancies in the surface of the TiO₂ structure yielding carriers type holes localized in the 3d orbitals of Ti atoms.

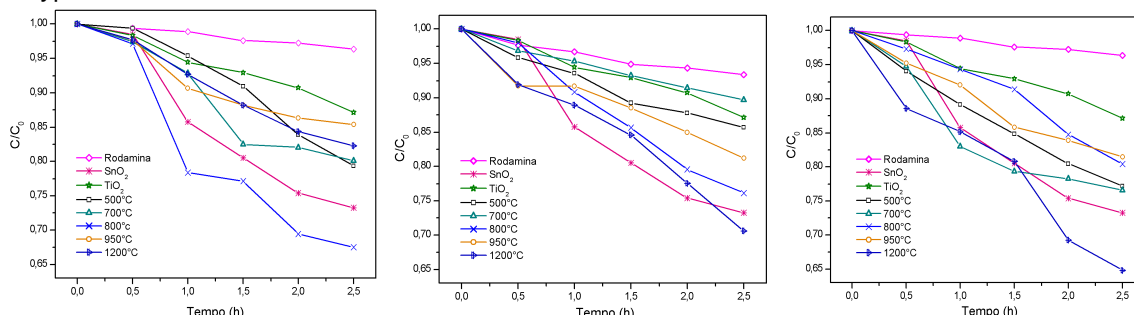


Figure 1: Dye Rhodamine B photodegradation for the SnO₂-TiO₂ system

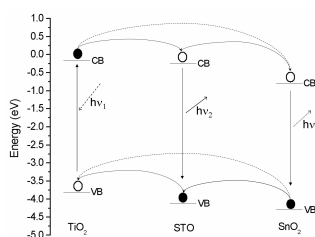
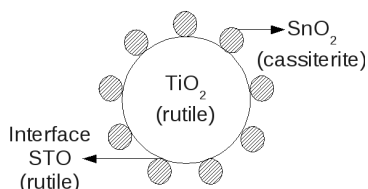


Figure 2: Illustration of the Sn_xTi_{1-x}O₂ interface (a) and electronic levels among SnO₂-TiO₂ system.

References

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