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Mesoporous BiVO4 Thin Films as Efficient Visible Light Driven Photocatalyst

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Abstract : Photocatalytic processes play key role in the production of a new source of energy (as hydrogen), design of self-cleaning surfaces or for the environment preservation. The most challenging task deals with the purification of water distinguished by high efficiency. In the mentioned process, organic pollutants in solutions are decomposed to the simple, non-toxic compounds as H2O and CO2. The most known photocatalytic materials are ZnO, CdS and TiO2 semiconductors with a particular involvement of TiO2 as an efficient photocatalysts even with a high band gap equal to 3.2 eV which exploit only UV radiation from solar emitted spectrum. However, promising material with visible light induced photoactivity was searched through the monoclinic polytype of BiVO4 which has energy gap about 2.4 eV. As required in heterogeneous photocatalysis, the high contact surface is required. Also, BiVO4 as photocatalyst can be optimized by increasing its surface area by achieving the mesoporous structure synthesize. The main goal of the present work consists in the synthesis and characterization of BiVO4 mesoporous thin film. The synthesis method based on sol-gel was carried out using a standard surfactants such as P123 and F127. The thin film was deposited by spin and dip coating method. Then, the structural analysis of the obtained material was performed thanks to X-ray diffraction (XRD) and Raman spectroscopy. The surface of resulting structure was investigated using a scanning electron microscopy (SEM). The computer simulations based on modeling the optical and electronic properties of bulk BiVO4 by using DFT (density functional theory) methodology were carried out. The semiempirical parameterized method PM6 was used to compute the physical properties of BiVO4 nanostructures. The Raman and IR absorption spectra were also measured for synthesized mesoporous material, and the results were compared with the theoretical predictions. The simulations of nanostructured BiVO4 have pointed out the occurrence of quantum confinement for nanosized clusters leading to widening of the band gap. This result overcame the relevance of nanosized objects to harvest wide part of the solar spectrum. Also, a balance was searched experimentally through the mesoporous nature of the films devoted to enhancing the contact surface as required for heterogeneous catalysis without to lower the nanocrystallite size under some critical sizes inducing an increased band gap. The present contribution will discuss the relevant features of the mesoporous films with respect to their photocatalytic responses.

Keywords : bismuth vanadate, photocatalysis, thin film, quantum-chemical calculations
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