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TUNING THE OPTICAL, ELECTRICAL AND PHOTOELECTROCATALYTIC PROPERTIES OF ZNO MATERIALS BY VARYING OF INTRINSIC DEFECTS CONCENTRATION

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During the last decade zinc oxide (ZnO) has attracted considerable attention as a promising material for electronic, optoelectronic and spintronic devices. ZnO has a wide bandgap (3.37 eV at room temperature) and relatively large exciton binding energy (60 meV) which enables multifunctional application. Until now ZnO-based materials have been used as UV and blue light emitters, varistors, thermistors, semiconductors, photoanodes, and other. Various approaches have been applied to improve functional properties of zinc oxide, such as: fabrication of ZnO-based heterojunction particles, particles' surface sensitization, hydrogenation, etc. It has been found that intrinsic defects (vacancies, interstitials and antisites) in the crystal structure of a ZnO strongly influenced its electrical and optical properties. Thus, correlation of the intrinsic defects concentration with optical and electrical properties of ZnO materials is of great importance for their further application in opto-electronic devices.
In this study we investigated the influence of intrinsic defects concentration on the optical, electrical and photoelectrocatalytic properties of ZnO materials. To obtain ZnO powder with a high concentration of intrinsic defects microwave processing of precipitate was employed, while for further varying of defects concentration, the powder was thermally treated in three different atmospheres: air, argon and oxygen. The ZnO powder was uniaxially pressed (P = 100 MPa) in cylindrical compacts (∅ 6 mm and $h \approx 3$ mm) which were sintered in different atmospheres by heating rate of 10 °/min up to 1100 °C, and with dwell time of 1 h. To study a crystal structure of ZnO samples XRD and Raman spectroscopy were used, while for microstructural investigation field emission scanning electron micrographs were recorded. Optical properties were studied using UV–Vis diffuse reflectance spectroscopy. To reveal the role of intrinsic defects in ZnO crystal lattice on functional properties, XPS, photoluminescence, electroluminescence and electrochemical impedance spectra were analyzed. A detailed analysis of the experimental results imply that a high concentration of intrinsic defects, in particular oxygen vacancies, is of the greatest importance for tunable light-emitting diode application and significant for the photoanode properties. To support our experimental observation we performed *ab initio* calculations based on density functional theory (DFT).

SYNTHESIS AND CHARACTERIZATION OF ANATASE-BROOKITE TIO_2 NANOPARTICLES IN PRESENCE OF MCAA

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TiO_2 is well known as a superior material semiconductor. Nevertheless, TiO_2 as catalyst still presents some limitations regarding the accumulation of electrons in the conductive band that leads to recombination of the photoexcited electron-hole pairs during the Advance Oxidation Process-AOP. Furthermore, the extended band-gap energy (3.2 eV) is possible to reduce it in order reach the visible ligth spectrum for improving its photocatalytic activity. Three different crystal forms exist. Anatase, Rutile, and Brookite. However, reports from brookite phase are still scarce. The Anatase-Brookite