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**Influence of point defects concentration on optical
and photocatalytic properties of ZnO ceramics**

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Zinc oxide is one of the most studied materials due to its wide bandgap (3.37 eV) and large exciton binding energy (60 meV) which enables application in electronics, optoelectronics and spintronics. In the forms of single crystal and thin-film ZnO are used as UV and blue light emitter, while sintered ZnO-based ceramics are important as varistors, thermistors or semiconductors. It has been found that point defects in the crystal structure of a ZnO strongly influenced its electrical and optical properties. Neutral oxygen vacancies are considered to be a major component of the defect structure of ZnO. Thus, correlation of the oxygen vacancies concentration with band gap energy of ZnO product is important to its application in opto-electronic devices.

In this study we investigated the influence of point defects concentration in ZnO crystal structure on its optical and photocatalytic properties. We analyzed ZnO powders prepared by different techniques: (a) microwave processing of precipitate and (b) hydrothermal processing, which yield different ordered crystal structure. To increase a concentration of the point defects in the crystal structure, the powders were sintered in air atmosphere by heating rate of 10 °/min up to 1100 °C, with dwell time of 1 h. The crystal structure, average crystallite size and phase purity of the ZnO ceramics were determined by X-ray diffraction and Raman spectroscopy. The optical properties, in particular, absorption capacity and band gap energy, were studied using UV-Vis diffuse reflectance spectroscopy. To reveal the role of microstructures and point defects in ZnO crystal lattice, which are receptive for luminescence and photocatalytic activity of this functional oxide, photoluminescence (PL), photoluminescence excitation (PLE) and EPR spectra were analyzed. The influence of point defects concentration in the ZnO crystal structure on photocatalytic properties was examined via decolorization of methylene blue under direct sunlight irradiation. Correlation between amount of the point defects, absorption capacity and photocatalytic efficiency were established. In order to clarify the experimental results *ab initio* calculations based on density functional theory (DFT) were performed