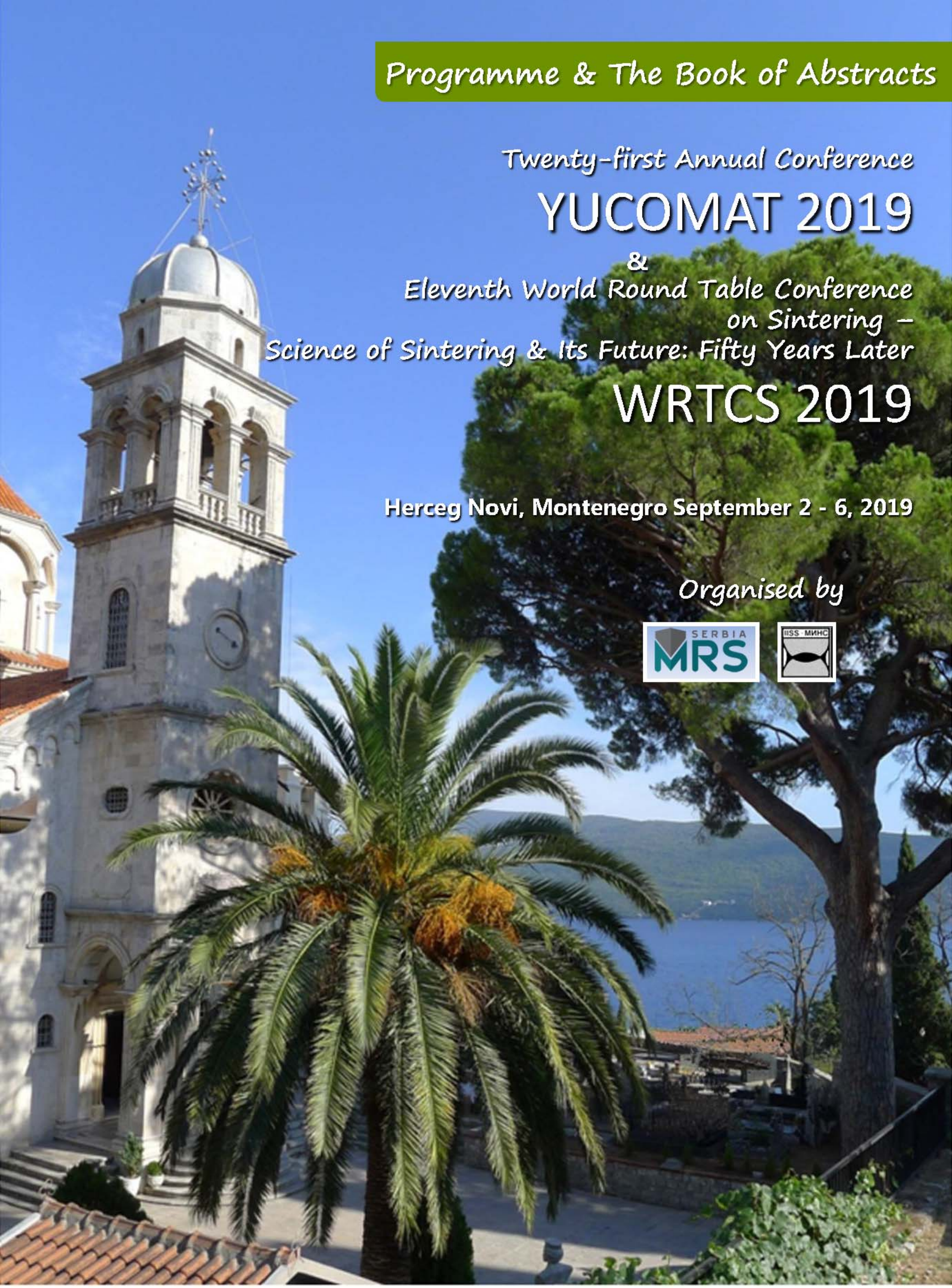

Programme & The Book of Abstracts

Twenty-first Annual Conference

YUCOMAT 2019

&

Eleventh World Round Table Conference on Sintering –
Science of Sintering & Its Future: Fifty Years Later

WRTCS 2019

Herceg Novi, Montenegro September 2 - 6, 2019

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Point defect-enhanced optical and photoelectrochemical water splitting activity of nanostructured $Zn_{1-x}Fe_yO_{(1-x+1.5y)}$

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Even has been under study since 1935, zinc oxide (ZnO) based materials still attract a huge scientific attention. Owing to a wide band gap energy (3.37 eV at room temperature) and a large exciton binding energy (60 meV) ZnO has a variety of application, e.g. in electronics, optoelectronics, spintronics and photocatalysis. Besides, it has been shown that zinc oxide-based materials have a great potential as photoelectrocatalysts in the processes of water splitting, yielding an increased both photocurrent density and photoconversion efficiency. However, with a band gap energy of 3.37 eV, ZnO is restricted to absorb UV light only. This restriction can be overcome by modifying optical properties of zinc oxide particles. During the years different approaches have been applied to modify the visible light photocatalytic activity of ZnO materials, for example: (1) metal and nonmetal ion doping, (2) hydrogenation, (3) the incorporation of crystalline defects in the form of vacancies and interstitials, (4) the modification of particles morphology and surface topology, etc.

In this study we employed 3d metal ion substitution to improve visible light-driven photoactivity of zinc oxide particles. We investigated the influence of Fe concentration in $Zn_{1-x}Fe_yO_{(1-x+1.5y)}$ nanoparticles on crystal structure, textural, optical and photoelectrocatalytic properties. $Zn_{1-x}Fe_yO_{(1-x+1.5y)}$ nanoparticles with nominally 5, 10, 15 and 20 at.% of Fe ions were synthesized by microwave processing of a precipitate. The crystal structure and phase purity of the samples were investigated by X-ray diffraction, Raman and ATR-FTIR spectroscopy. Mössbauer spectroscopy was carried out to clarify the valence state of the iron ions in the ZnO crystal structure. Effects of the iron ions concentration on particles morphology and texture properties were observed with field emission scanning electron microscopy (FE–SEM), transmission electron microscopy (TEM) with elemental mapping, and nitrogen adsorption–desorption isotherm, respectively. The optical properties were studied using UV–Vis diffuse reflectance and photoluminescence (PL) spectroscopy. Photoelectrochemical activity of the $Zn_{1-x}Fe_yO_{(1-x+1.5y)}$ samples as anode material was evaluated by linear sweep voltammetry in Na_2SO_4 electrolyte; the oxygen evolution kinetics were determined and compared. In addition, a series of first principles calculations were performed to address the influence of the iron concentration on the electronic structure of $Zn_{1-x}Fe_yO_{(1-x+1.5y)}$ samples.

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