3rd International Meeting

on

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September 25-26, 2018, University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia

BOOK OF ABSTRACTS

BELGRADE, SERBIA 2018

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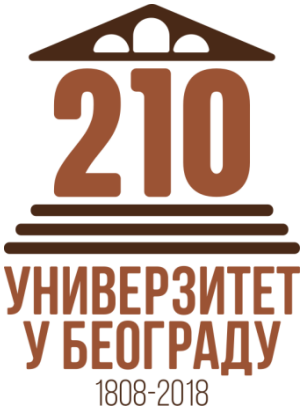

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EXPERIMENTAL AND THEORETICAL INSIGHTS ON CHARGE TRANSFER AND CLUSTER FORMATION IN CO-DOPED N-TiO_2

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Inroduction

Among various applications of TiO_2, hydrogen generation from methanol/ethanol solutions or ultimately water, is one of the big interest for renewable energy applications. One of approaches in modifying properties of titania in order to bring this cheap material one step closer to these applications is oxide doping and co-doping as a way of stimulating charge transfer between the metal and oxide surface [1]. We consider charge transfer and optical properties of doped and co-doped TiO_2 surfaces, as well as deposition of platinum and palladium at the 001 anatase TiO_2 surface, to study influence of nitrogen doping on metal clustering and metal-support interaction.

Methods

Nanosized N-doped TiO_2 is synthetized from titanium(IV) isopropoxide and urea as nitrogen source. Palladium and platinum are deposited at the surface of N/TiO_2 particles by photo-reduction from the chloride solutions. Diffuse reflectance spectra (DRS) and XPS spectra of N-TiO_2 as well as Pd,N/TiO_2 and Pt,N/TiO_2 are recorded in order to study optical properties of co-doped TiO_2 and charge state of deposited metals.

Nitrogen doping and formation of Pt and Pd dimers on 001 anatase surface, as well as combination of both, is studied using spin-unrestricted DFT-based calculations within general gradient approximation (PBE-GGA) and pseudopotential plane wave approach (Vanderbilt-type ultrasoft pseudopotentials), as implemented in the Quantum ESPRESSO package.

Results

Studied materials have a dominant structure of the anatase phase, with a small percentage of the rutile phase (3.8%). DRS spectra show significant shift of the absorption edge towards the longer wavelengths as compared to the pure TiO_2. The band gap is reduced from 3.15 eV for commercial anatase TiO_2 to 2.40 eV for N-TiO_2 and 2.35 eV for both Pt/N-TiO_2 and Pd/N-TiO_2[2]. XPS is used to study electronic structure and charge state of atoms at the surface of nanoparticles. Top of the valence zone of the reference