The Serbian Society for Ceramic Materials
Institute for Multidisciplinary Research (IMSI), University of Belgrade
Institute of Physics, University of Belgrade
Center of Excellence for the Synthesis, Processing and Characterization of Materials for use in Extreme Conditions "CEXTREME LAB" - Institute of Nuclear Sciences "Vinča", University of Belgrade
Faculty of Mechanical Engineering, University of Belgrade
Center for Green Technologies, Institute for Multidisciplinary Research, University of Belgrade
Faculty of Technology and Metallurgy, University of Belgrade
Faculty of Technology, University of Novi Sad

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Branko Matović
Zorica Branković
Aleksandra Dapčević
Vladimir V. Srdić

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5CSCS-2019

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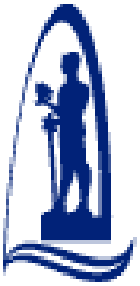

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NOVEL APPROACH TO DOPANT TREATMENT IN ELECTRONIC STRUCTURE CALCULATIONS – A CASE STUDY OF Mg-DOPED ZINC OXIDE

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A commonly used method for modifying a crystal is doping, where a portion of lattice positions occupied by an element in a structure is taken up by another element (dopant). It is therefore important to determine how doping a crystal influences its stability. Zinc oxide is a semiconductor with wide spectrum of potential application – LEDs, gas sensors, battery anodes, and even more when doped – changing its magnetic, electrical or optical properties by doping opens possibility for other applications like in spintronics.

In order to examine the influence of dopant on stability, we have decided to observe magnesium-doped zinc oxide in a computational model. Using isovalent dopant makes the study simpler, and Mg-doped ZnO has been extensively studied in theory and experiment, which makes it a good basis to compare our findings to previous studies. We assumed that periodic dopant placement would contribute to lower energy of the system compared to a random dopant placement, thus we decided to use a supercell model periodically replicated in 3D space. This approach can indicate whether formation of superstructures can be expected in experiment based on enthalpic contribution of the periodically placed dopant. Our model supercell is made of eight unit cells (2×2×2) with one zinc (6.25 at.%) replaced with magnesium. Using linearized augmented planewave (LAPW) method in combination with quantum theory of atoms in molecules (QTAIM), our aim is to determine energy contribution of a zinc atom in the pure zinc oxide structure and that of magnesium replacing zinc in the doped supercell in order to show how doping contributes to stability of the crystal structure. The goal of this combined approach is to go beyond thermodynamics expressed in terms of simple energy differences. Using unique and physically meaningful partition of unit cell space it is possible to calculate various integral contributions (charge density, energy) of dopant embedded at the particular atomic site. The precise electronic structure is determined using methods that extend beyond DFT, like LDA+U Hubbard approach and hybrid functionals for exact description of exchange term in the Hamiltonian of the system.