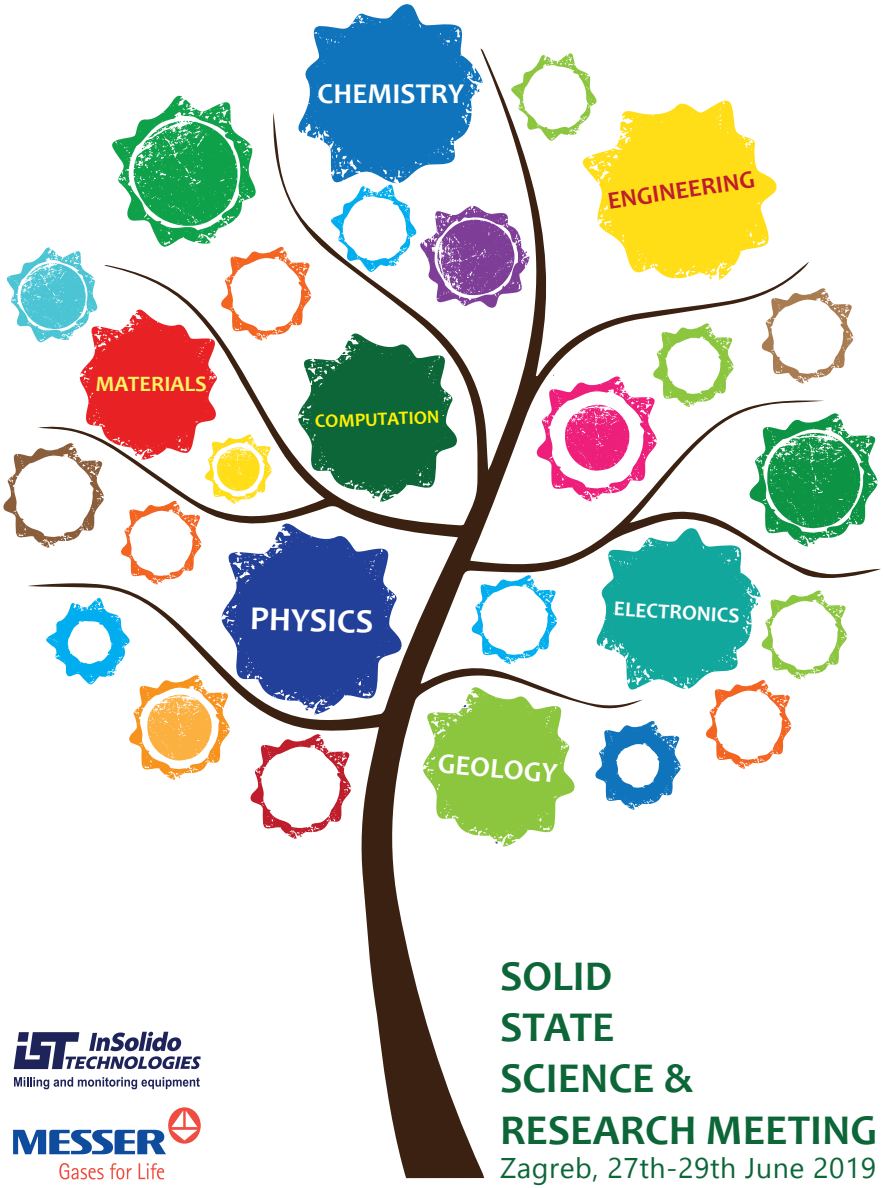

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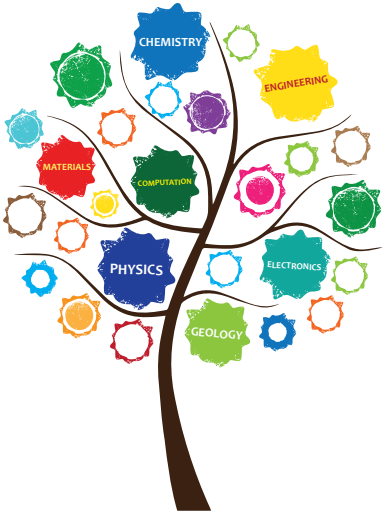

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P56: Bonding nature in Mg doped ZnO system - charge density topology approach

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Doping of semiconductors is commonly used for tailoring electrical, magnetic, optical and structural properties of ceramic materials. Understanding the effect of doping on stability of the material is important in order to improve the process and obtain targeted properties. Commonly used approach for determining energy contribution of doping is based on comparing the heat of formation of doped and undoped crystals. Our idea is to go beyond this thermodynamic approach and determine energy contribution of each particle in bulk structure.

Doped zinc oxide has been a subject of many studies concerning doping, and this makes it a good choice to compare our results to pervious findings. Magnesium as an isovalent dopant makes the model simpler for computation, and Mg-doped zinc oxide has been previously studied in both theory and experiment. Our assumption was that periodic placement of dopants would lower the energy of the system compared to a random placement of dopants. Therefore, a supercell model replicated in 3D space has been used. The model is made of eight unit cells (2×2×2) with a single zinc replaced with magnesium (6.25 at%). Our aim is to determine energy contribution of both, a zinc in pure zinc oxide structure and of magnesium in doped supercell. We combined linearized augmented planewave (LAPW) method with quantum theory of atoms in molecules (QTAIM). This approach enables us to determine the effect of doping on stability of the structure. Various 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 are used to determine precise electronic structure, while QTAIM-based partition of supercell space allows us to calculate various integral contributions (charge density, energy) of each particle taking any site in the supercell.