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Unveiling the Impact of Ultra High Vacuum Annealing Levels on Physico-Chemical Properties of Bulk ZnSe Semiconductor

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Abstract : In this current paper, our aim work is to link as possible the obtained simulation results and the other experimental ones, just focusing on the electronic and optical properties of ZnSe. The predictive spectra of the total and partial densities of states using the Full Potential Linearized/Augmented Plane Wave method with the newly Tran-Blaha (TB) modified Becke-Johnson (mBJ) exchange-correlation potential (EXC). So the upper valence energy (UVE) levels contain the relative contribution of Se-(4p and 3d) states with considerable contribution from the electrons of Zn-2s orbital. The dielectric function of w-ZnSe, with its two parts, appears with a noticeable anisotropy character. The microscopic origins of the electronic states that are responsible for the observed peaks in the spectrum are determined through the decomposition of the spectrum to the individual contributions of the electronic transitions between the pairs of bands, where Vi is an occupied state in the valence band, and Ci is an unoccupied state in the conduction band. X-PES (X Ray-Photo Electron Spectroscopy) is an important technique used to probe the homogeneity, stoichiometry, and purity state of the title compound. In order to check the electron transitions derived from simulations and the others from Reflected Electron Energy Loss Spectroscopy (REELS) technique which was of great sensitivity, is used to determine the interband electronic transitions. In the optical window (Eg), all the electron energy states created were also determined through the specific gaussian deconvolution of the photoluminescence spectrum (PLS) that probed under a room temperature (RT).

Keywords : spectroscopy, WIEN2K, IIB-VIA semiconductors, dielectric function
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