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DFT CALCULATIONS ON ELECTRONIC PROPERTIES OF ZNO THIN FILMS DEPOSITED BY SPRAY PIROLYSIS.

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Introduction - Thin films of Zinc oxide (ZnO) has a wide range of technological applications, as transparent conducting electrodes in solar cells, flat panel displays, and sensors, for example. More recently applications in optoelectronics, like light emitter diodes and laser diodes, due to its large band gap, are been explored. Studies of ZnO thin films are important for these applications. Methodology - In this study thin films of ZnO have been deposited by spray pirolysis on glass substrate. The films were characterized by XRD and UV-VIS techniques and the electronic properties as a function of the film thickness have been investigated by DFT calculations with B3LYP hybrid potential implemented in the CRYSTAL09 code. Results - The difractograms obtained for the ZnO thin films as a function of the thickness are shown. The films exhibit a hexagonal wurtzite structure with preferred c-axis orientation in (002) direction of ZnO crystal. A quantum mechanical approach based on the periodic Density Functional Theory (DFT), with B3LYP hybrid potential was used to investigate the electronic structure of the films as a function of the thickness. The CRYSTAL09 code has been used for the calculations on the wurtzite hexagonal structure of ZnO - spatial group P63mc. For optimizing the geometry of the pure ZnO crystal, the experimental lattice parameters were got as follows: a= 0.325 nm, b= 0.325 nm, c= 0.5207 nm with c/a= 1.602. Considering to the calculations of the band structure, it is suggested that the semiconducting properties of ZnO arises from the overlapping of the 4s orbital of the conducting band of Zn and the 2p orbital of the top of valence band of O. Conclusions - The structure of ZnO thin film deposited on glass substrate present preferential orientation in (002) direction. Variation in the optical properties as a function of the film thickness was observed. The band gap energy was determined from optical analysis to be ~3.27 eV. The refractive index decreased monotonically as a function of time thermal treatment of 2.01 at 1.97 determined at 632.8 nm. The results are comparable with others previously obtained.