Investigation of Properties of ZnO Nanostructures by First- Principals Calculations

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Abstract : Structural and microstructural properties were investigated by first-principals computing. The ZnO powder as Transparent Ceramics exhibited a hexagonal crystal structure with space group p63mc of ZnO. We applied the present first-principals approach to the electronic structure of the ZnO structures. Band structure and density of states of the phase of crystal ZnO computed using first principal methods, confirmed that pure ZnO is a direct band gap semiconductor when obtained in the B4 type structure phase.

Keywords : ZnO;DFT; FP-LAPW