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A Study on ZnO Nanoparticles Properties: An Integration of Rietveld Method and First-Principles Calculation

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Abstract : Zinc oxide (ZnO) has been extensively used in optoelectronic devices, with recent interest as photoanode material in dye-sensitize solar cell. Numerous methods employed to experimentally synthesized ZnO, while some are theoretically-modeled. Both approaches provide information on ZnO properties, but theoretical calculation proved to be more accurate and timely effective. Thus, integration between these two methods is essential to intimately resemble the properties of synthesized ZnO. In this study, experimentally-grown ZnO nanoparticles were prepared by sol-gel storage method with zinc acetate dihydrate and methanol as precursor and solvent. A 1 M sodium hydroxide (NaOH) solution was used as stabilizer. The optimum time to produce ZnO nanoparticles were recorded as 12 hours. Phase and structural analysis showed that single phase ZnO produced with wurtzite hexagonal structure. Further work on quantitative analysis was done via Rietveld-refinement method to obtain structural and crystallite parameter such as lattice dimensions, space group, and atomic coordination. The lattice dimensions were a=b=3.2498Å and c=5.2068Å which were later used as main input in first-principles calculations. By applying density-functional theory (DFT) embedded in CASTEP computer code, the structure of synthesized ZnO was built and optimized using several exchange-correlation functionals. The generalized-gradient approximation functional with Perdew-Burke-Ernzerhof and Hubbard U corrections (GGA-PBE+U) showed the structure with lowest energy and lattice deviations. In this study, emphasize also given to the modification of valence electron energy level to overcome the underestimation in DFT calculation. Both Zn and O valance energy were fixed at Ud=8.3 eV and Up=7.3 eV, respectively. Hence, the following electronic and optical properties of synthesized ZnO were calculated based on GGA-PBE+U functional within ultrasoft-pseudopotential method. In conclusion, the incorporation of Rietveld analysis into first-principles calculation was valid as the resulting properties were comparable with those reported in literature. The time taken to evaluate certain properties via physical testing was then eliminated as the simulation could be done through computational method.

Keywords : density functional theory, first-principles, Rietveld-refinement, ZnO nanoparticles
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