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$DMol_3$ Calculation of Electronic Properties of ZnO with different LDA approximation

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Abstract : ZnO is a II-IV semiconducting material having band gap 3.37 eV at room temperature. It has been good interest in recent years due to the wide application of ZnO in laser, Green-Blue LED, solar cell, robotic etc. Applying the first principle DFT we can calculate various properties of ZnO like lattice constant, band plot, magnetic properties and optical properties etc. In this work DFT *first-principle* calculation using $DMol_3$ code with LDA-PWC and LDA- VWN approximation for electronic structure calculation of ZnO performed and compared both the result with experimental data. DOS and PDOS plotted and analyzed for both functional.

Keywords: ZnO, DFT, $DMol_3$, LDA-PWC, LDA-VWN, DOS, PDOS