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An Insight to origin of ferromagnetism in ZnO and N implanted ZnO thin films: Experimental and DFT approach

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In the present study, we have elucidated an effective way to simultaneously tune the optical bandgap and magnetic properties of zinc oxide (ZnO). This can be achieved by the incorporation of nitrogen ions via any means in the host matrix. On a broader way, we have systematically investigated the influence of N ions in ZnO thin films through experimental techniques and density functional theory (DFT) calculations to understand the physical mechanism governing the observed magnetic behaviour and variation in bandgap. For this, RF sputtered ZnO thin films deposited over Si substrates were implanted with N ions by varying the fluences and studied for their optical and magnetic properties. The pristine ZnO films is having saturation magnetization of ~ 2.45 emu/cm³ which becomes almost twice compared for the fluence of 1×10^{17} ions/cm². Furthermore, the optical bandgap is tuned from 3.27 eV to 3.04 eV with N ion fluences. Our work signifies the new insight to understand the basis of ferromagnetism in non-magnetic ions doped ZnO system.

Keywords: Ion implantation, bandgap tuning, defects induced magnetism, first principle calculations.

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