

## Study of Active Surface Defects in *Ti* Doped *ZnO* Nanoparticles

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**Abstract.** The effects of surface defect (oxygen vacancies) on the electronic structure and photoluminance properties of the titanium doped ZnO nanoparticles are investigated in this paper. Nanoparticle of different sizes ranging from 6 to 25nm were characterized by x-ray diffraction (XRD), Transmission electron micrograph, x-ray photoemission emission spectroscopy (XPS) and photoluminescence (PL) spectra. Structural analysis (including XRD, TEM and HR-TEM) and electronic studies (via XPS) indicate that the Ti ions are well substituted for the Zn ions in the ZnO matrix. Surface defects (oxygen vacancies) systemically increase, as manifested by the Zn2p core level of XPS measurements, with decreasing particles size and it further confirmed via Raman scattering measurements. The intensity of the visible peak in PL spectra exhibits an apparent non-monotonic change over the entire range of particle size. It is found that the intensity first decreases with increasing particle size but increases above a typical size. This non-monotonic profile of visible intensity could be explained via two different mechanisms, where intensity changes from being followed by hole-trapped tunneling in lower size particles [1] to being followed by increasing surface depletion region [2], containing rich amount of doubly charged oxygen vacancy ( $V_o^{2+}$ ), in the bigger size particle.

### References

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