

Interconnection of Charge Neutrality Level with Electronic Structure and P-D Hybridization and its Modification upon Electronic Excitations

Arkaprava Das^{1*}, Subodh K. Gautam¹, G. R. Umapathy¹, S. Ojha¹, Fouran Singh¹ and D. K. Shukla²

¹Inter University Accelerator Centre, India

²UGC-DAE Consortium for Scientific Research, India

Undoped and tin doped cadmium oxide (CdO) based thin films are irradiated by 84 MeV Si⁶⁺ and 120 MeV Ag⁹⁺ ions. In the present work the charge neutrality level (CNL) [1] in highly conducting CdO thin films is demonstrated by the observed variation in the band gap upon annealing and doping. The increase in crystallite size with tin doping is a signature of decrease of CdO stoichiometry by substitutional replacement of Cd with Sn. Each Cd²⁺ ions are substituted by Sn²⁺ ions with reduction of Sn⁴⁺ via creating oxygen vacancies in the lattice which also enhances the carrier concentration in the tin doped thin film [2]. The band gap enhancement cannot be explained by Burstein-Moss Shift (BMS) only but can be explained by formation of charge neutrality level (CNL). The level of local CNL resides at the branch point of virtual gap states (ViGS) generation of which is the consequence of tin doping in CdO lattice. Further investigations using soft x-ray absorption spectroscopy (SXAS) at Oxygen *k* and Cadmium *M*_{4,5} edge and the analysis of the spectral features has revealed an evidence of *p-d* interaction between O *2p* and Cd *4d* orbitals. After irradiation, the thin films exhibit an unusual band gap enhancement *via* generation of oxygen vacancies due to huge electronic energy deposition inside the lattice by Ag and Si ions. The observed band gap enhancement has been substantiated by a schematic block diagram.