Optical properties of Nitrides and Oxides based semiconductor : A first principle study

Sudhir Kumar* [1]

[1] *Applied Physics Department, Faculty of Engineering and Technology, Mahatma Joyotiba Phule Rohilkhand University, Bareilly -243 006, INDIA*

ABSTRACT

The nitrides and oxides based semiconductors are getting importance due to their technological applications. In the first part of my talk, the predicated optical properties for the In-rich and As-rich ternary alloys will be discussed. The obtainded results will be also explained in contrast to available measured data's. InN plays a central role because of it ability to make stable alloys with AlN and InAs which cover a wide range of the energy band gap say 0.32 eV to 6.2 eV. In the second part of the talk, I shall present some recent findings related to wide band gap oxide semiconductors like SnO_2, Ga_2O_3 and In_2O_3. These are n-type of transparent conducting oxides (TCO's) widely used by industries as transparent electrodes. In these materials, the direct optical transitions from valence band maxima to conduction band minima are dipole forbidden and therefore optical absorptions occur only at higher than the measured energy band gap. The calculated results will be discussed alongwith available state of art theoretical spectroscopic techniques and experimental results

State of the art techniques like full potential linear augmented plane wave method (FP-LAPW) and Vienna ab-intio Simulation Package (VASP) based on the density functional theory alongwith local density approximation modified Beck Jhonson potential is used for the optical properties. However, local density approximation(LDA) and generalised gradient approximation(GGA) are still one of the best option available for the structural parameters

*Otto-von-Guericke-University Magdeburg, Faculty of Natural Sciences, Institute of Experimental Physics, Department of Experimental Physics/Material Physics, Universitätsplatz 2 (Building 16) 39106 Magdeburg