Contribution ID: **222** Type: **Oral**

Structural, optical, electronic and magnetic properties of Fe-doped ZnO nanoparticles synthesized by combustion method and first-principles calculation

Thursday, 25 May 2017 16:30 (15 minutes)

In this work, $Zn_{1-x}Fe_xO$ (x=0.000, 0.0625 and 0.125) materials have been investigated in both experimental and theoretical aspects. The pure and Fe-doped ZnO nanoparticles were prepared by a combustion method. The crystal structures were characterized using the X-ray diffraction (XRD), morphology by the transmission electron microscopy (TEM) techniques, magnetic behavior by vibrating sample magnetometer (VSM), and optical band gap by ultraviolet-visible (UV-Vis) spectroscopy. In first-principles calculation, density of states (DOS) and electronic band structure of the $Zn_{1-x}Fe_xO$ supercell have been calculated using general gradient approximation with Hubbard model scheme (GGA+U), packaged in the Vienna Ab initio Simulation Package (VASP). The calculation was performed using self-consistent projected augmented plane wave (PAW). From the study, the prepared nanoparticles of pure ZnO and 6.25 and 12.5% by mole of Fe-doped ZnO show different magnetic behavior from diamagnetism of ZnO. In the presence of the calculation results, the density of states of dopant systems shows state difference of spin up and spin down electron also an intermediate band, induced by d orbital of iron atoms, located near the valence band is observed. From these, it's interesting that small amount of iron doping can engineer the band structure, and induce both intermediate band and magnetism in nonmagnetic ZnO material.

Primary authors: Ms SIKAM, Pornsawan (Khon Kaen university); Dr MOONTRAGOON, Pairot (Khon Kaen University); Mr JUMPATAM, Jutapol (Khon Kaen University); Dr PINITSOONTORN, Supree (Khon Kaen University); Dr THONGBAI, Prasit (Khon Kaen University); Dr KAMWANNA, Theerasak (khon Kaen University)

Presenter: Ms SIKAM, Pornsawan (Khon Kaen university)

Session Classification: A16: Magnetic and Semiconductor

Track Classification: Magnetic and Semiconductor Physics