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## Room temperature ferromagnetism in various non-magnetic oxides

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A *b-initio* calculations on the possibility of room temperature ferromagnetic ordering in non-magnetic oxides have been performed by doping various p-block elements X (X=B, C, N, Al, Si, P, S, Ga, Ge and As) in ZnO, TiO<sub>2</sub>, MgO, SnO<sub>2</sub> etc. The spin-polarized density of states calculation has been performed using the code MedeA VASP for all the structures with two same p-block elements, doped at oxygen sites. A significant amount of induced magnetic moment has been observed in some cases. The sources of magnetism are np orbital electrons of the dopants along with the 2p orbital electrons of neighboring oxygen atoms. Among them, stable ferromagnetic (spin triplet) ordering states have been identified and the theoretical calculations have been verified by experiments. The room temperature ferromagnetic properties of various semiconducting oxides can be useful for spintronics applications in future. A detailed result of spin-spin interaction study along with our experimental observations for room temperature ferromagnetism in different systems will be presented.



Figure 1: Local magnetic density distribution for P doped SnO<sub>2</sub>. The source of magnetism is the P-atom doped at O-site in SnO<sub>2</sub>.

## **Recent Publications**

- 1. Luitel H et al. (2016) Positron annihilation lifetime characterization of oxygen ion irradiated rutile TiO<sub>2</sub>. Nuclear Instruments and Methods B. 379:215-218.
- Luitel H and Sanyal D (2017) *Ab initio* calculation of magnetic properties in B, Al, C, Si, N, P and As doped rutile TiO<sub>2</sub>. Int. J. Mod. Phys. B. 31:1750227.
- 3. Luitel H et al. () Defect generation and recovery in polycrystalline ZnO during annealing below 300°C as studied by *in situ* positron annihilation spectroscopy. J. Mat. Sc. 52:7615.
- 4. Luitel H Roy S and Sanyal D (2018) Ferromagnetism in P and As doped SnO<sub>2</sub>: first-principle study. Computational Condensed Matter. 14:36-39.
- 5. Sarkar A et al. (2017) Positron annihilation spectroscopic characterization of defects in wide band gap oxide. Semiconductors. Mat. Res. Exp. 4(3):035909.

## Biography

Homnath Luitel is a PhD student at Variable Energy Cyclotron Centre (VECC), a research institute in Kolkata. He has done his Post MSc course from the same institute and has registered for PhD program under Homi Bhabha National Institute (HBNI), Mumbai. His research area mainly focuses on room temperature ferromagnetism in various non-magnetic semiconducting oxides; and also dilute magnetic semiconductors, defects characterization, etc.

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