Department of Physics
Central University of Tamil Nadu
Thiruvarur-610 005

Ph. D. Pre-Submission Seminar

Name of the Student : Lokanath Patra, Research Scholar (Reg. No: R131403)
Name of the Supervisor : Prof. P. Ravindran, Department of Physics, CUTN
Title of the Thesis : First principles modelling of multiferroic materials with giant magnetoelectric coupling.
Date and Time : 26.10.2018 & 2.30 p.m.
Venue : Seminar Hall (GF), Department of Physics, CUTN.

Abstract

Materials with multifold functionalities such as ferroelectricity, magnetism[1,2], and ferroelasticity have been receiving everlasting attention due to miniaturization of sensors, development of multistate high-density storage technologies, and integration of multifunctional devices/systems[3,4]. One of the driving forces along these lines is an exploration of magnetoelectric (ME) multiferroic (MF) materials in which multifold ferroic functionalities i.e. (anti-)ferromagnetism and (anti-)ferroelectricity coexist and inter-coupled, resulting promising potential applications. But the co-existence of (anti)ferroelectricity and (anti)ferromagnetism is rare due to their opposing mechanisms of origin. In perovskite type materials (ABO_3), one possible way to combine these two order parameters is the introduction of lone- pair cation at the *A*-site which drives off-center displacement and partially filled "*d*" shell cations at the *B*-site which contributes to the magnetism[5,6] Though there exist many lone pair based magnetoelectric MFs, the coupling between the electric and magnetic degrees of freedom is weak in most of the cases and that prevents one to use them for practical applications. In lone pair based MFs, presence of d^n cations at the B-site with properties like spin-state transition, orbital ordering etc. can enhance the ME coupling abnormally[3,6]. With these starting ideas, we have designed new series of MF materials where two mechanisms for ferroelectricity ($6s^2$ lone-pair electrons, Ti^{4+} cations with d^0-ness) coexist, such as xBaTiO$_3$-(1-x)BiCoO$_3$[7], xPbTiO$_3$-(1-x)BiCoO$_3$[8], PbTi$_{1-x}$V$_x$O$_3$[9], Bi$_2$$XTiO_6$ (X = Mn, Fe, Ni)[10-12] along with magnetism from cation with partially filled 3d shell i.e. Fe^{2+}, Co^{3+}, V^{4+} etc. Our results show that these compounds have the tendency to show giant ME coupling i.e. the applied electric field can make magnetic-to-nonmagnetic transition and conversely a ferroelectric-to-paraelectric phase transition can be obtained by an external magnetic field. In this talk, I will discuss about the mechanism behind such strong coupling in the studied materials. This work demonstrates that the cooperative effect of strong lattice coupling with different order parameters on the ME properties would be important to develop next generation memory devices, sensors, magnetic switches etc.

References:

1. M.R. Ashwin Kishore, H. Okamoto, **Lokanath Patra**, R. Vidya, Anja O. Sjåstad, H. Fjellvåg, P. Ravindran, *Phys. Chem. Chem. Phys.* 18, 27885 (2016)
2. **Lokanath Patra**, M.R. Ashwin Kishore, R. Vidya, Anja O. Sjåstad, H. Fjellvåg, P. Ravindran, *Inorganic Chemistry* 55 (22), 11898-11907 (2016).
3. Eerenstein W, Mathur ND, Scott JF, *Nature*. 2006; 442(7104):759.
4. Cheong, Sang-Wook, and Maxim Mostovoy. *Nature materials* 6.1 (2007): 13-20.
5. P. Ravindran, R. Vidya, A, Kjekshus, H. Fjellvåg, O. Eriksson. *Physical Review B.* 2006 14; 74 (22): 224412.
6. P. Ravindran, R. Vidya, O. Eriksson, H. Fjellvåg, *Advanced Materials*, 2008 Apr 4;20(7):1353-6.
7. **Lokanath Patra**, Zhao Pan, Jun Chen, Masaki Azuma, P. Ravindran, *Phys. Chem. Chem. Phys.* (20), 7021-7032. (2018)
8. Zhao Pan, Jun Chen, **Lokanath Patra**, P. Ravindran et. al. Submitted to *Chemistry of Materials.*
9. **Lokanath Patra**, R. Vidya, H. Fjellvåg, and P. Ravindran, Submitted to *Inorganic Chemistry.*
10. **Lokanath Patra**, P. Ravindran, *AIP Conference Proceedings* 1832 (1), 130053 (2017)
11. **Lokanath Patra**, P. Ravindran, *AIP Conference Proceedings*, 1942 (1), 130054 (2017)
12. **Lokanath Patra**, P. Ravindran, *AIP Conference Proceedings*, 1953 (1), 120039 (2017).

All are welcome

Seminar Coordinators

Head of the Department