

## **CURRICULUM VITAE**

# **Dr. Zahid Ali**

Assistant Professor, Department of Physics  
University of Malakand, Chakdar Dir (L) Pakistan  
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### **Education:**

- Ph.D *Physics (2013)* Hazara University Mansehra, KP, Pakistan  
M.Sc *Physics (2004)* Department of Physics, University of Peshawar, KP, Pakistan  
B.Sc *Physics, Math (A), States (2002)* University of Peshawar, KP, Pakistan  
HSSc *Pre-Engg. (2000)* BISE Peshawar, KP, Pakistan  
SSC *Phy. Chem. Bio. Math, (1998)* BISE Peshawar, KP, Pakistan

### **HEC Approved Ph.D. Supervisor**

#### **Ph.D. Thesis Title:**

Investigations of Structural and Magnetic Properties of Cubic Perovskites by DFT

#### **Research Interest:**

Spintronics, Bandgap Engineering, Modeling of functional materials, Magneto-electronic, Optical, Thermoelectric and Mechanical Properties of solids by Density Functional Theory

### **Teaching Experiences (Government Sectors)**

- Lecturer Physics (Oct. 2011 to Jul. 2016): Department of Physics, University of Malakand, KP, Pakistan
- Lecturer Physics (Sep. 2010 to Jul. 2011): Department of Physics Hazara University Mansehra, KP, Pakistan
- Lecturer Physics (Oct. 2008-March 2009): Gov't Degree College Badh Bare, Peshawar, KP, Pakistan

### **Co-Curricular Experience**

- Semester coordinator in the Department of Physics, University of Malakand from Dec. 18, 2014 to present

### **International Workshops (Member Organizing Committee)**

- 1<sup>st</sup> International Workshop on Materials Modeling and Simulations (IWMMS 2011) held at University of Malakand (Pakistan) Sep. 07 to 11, 2011
- 2<sup>nd</sup> International Workshop on Materials Modeling and Simulations (IWMMS 2012) held at University of Malakand (Pakistan) May, 21 to 24, 2012.
- 3<sup>rd</sup> International Workshop on Materials Modeling and Simulations (IWMMS 2013) held at University of Malakand (Pakistan) July, 03 to 06, 2013.

### **National Conference (Secretary of the Conference/ Workshops)**

- National Workshop on Advanced Techniques on Materials Modeling and Simulations held at Center for Computational Materials Science, University of Malakand (Pakistan) Oct, 20 to 29, 2015.
- One-Day Conference on International Year of Light (IYL 2015) Organized by Center for Computational Materials Science and Department of Physics, University of Malakand in collaboration with National Institute of Lasers and Optronics (NILOP), Islamabad held at University of Malakand (Pakistan) Nov. 24, 2015

### **Papers/ Talk Present in Conferences/ Workshops**

- “Theoretical studies of SrTaO<sub>3</sub> by DFT+U” 2<sup>nd</sup> International Workshop on Materials Modeling and Simulations (IWMMS 2012) held at University of Malakand, Pakistan May, 21 to 24, 2012.
- “Magnetic structure of BaPrO<sub>3</sub> A-first principle study” International Conference on Condensed Matter Physics and Engineering” Dec. 27-29, 2012 held at Bahauddin Zakariya University, Multan, Pakistan
- “DFT Flavors and Applicability” DFT workshop at PINSTECH, held at PINSTECH, Islamabad, Pakistan dated Nov. 04-06, 2015

## Workshop Attended

- International Scientific Spring 2010 (ISS-2010) held at National Centre For Physics, Islamabad, Dated March 01-06, 2010
- DFT workshop at PINSTECH, held at Nilore Islamabad dated Sep. 23-25, 2014
- Indigenous On-Campus Training Workshop of Administrative Staff on “Semester bye-laws” held at University of Malakand, Pakistan; March 19 to 20, 2015.
- DFT workshop at PINSTECH, held at PINSTECH, Islamabad dated Nov. 04-06, 2015

## M. Phil Students Supervised

1. Mr. Abdul Sattar “DFT Studies of  $\text{AOsO}_3$  (A=Ca, Sr and Ba) Perovskites”
2. Mr. Rahm Zeb “Structural, Elastic, Electronic and Magnetic Studies of  $\text{TlTf}_3$  (T=Fe, Co and Ni)”
3. Mr. Mazhar Rahman “ab-initio Studies of Double Perovskites  $\text{LiMMoO}_6$  (M = Nb, Ta and Mo = W, Mo) by Modified Becke-Johnson Potential”
4. Mr. Israrullah “Theoretical studies of structural, electronic and magnetic properties of aluminum-rich intermetallic alloy  $\text{Al}_{13}\text{Fe}_4$ ”
5. Mr. Muhammad Sadiq “First principle studies of Mg-rich intermetallic  $\text{NdNiMg}_5$ ”
6. Mr. Noor Ullah “Theoretical studies of  $\text{Y}_2\text{M}_2\text{O}_7$  (M = Ti, V and Nb) pyrochlores”
7. Mr. Muhammad Ayoub “Variation in the physical properties of  $\text{La}_{0.5}\text{Ba}_{0.5}\text{CoO}_3$ ,  $\text{LaBaCo}_2\text{O}_{5.5}$  and  $\text{LaBaCo}_2\text{O}_6$ ”
8. Mr. Shahid Mehood “Theoretical studies of  $\text{SrFe}_x\text{Co}_{1-x}\text{O}_3$  (X= 0.25, 0.5, 0.75 and 1)
9. Mr. Rahman Zada “Hybrid DFT Studies of Inverse Perovskites  $(\text{Ln}_3\text{N})\text{Sn}$  (Ln = La, Ce, Pr, Nd and Sm)

## Publications:

1. **Zahid Ali**, I. Khan, M. Rehman, I. Ahmad, R. Ahmad, *Electronic Structure of the LiAA'O6 (A = Nb, Ta, and A' = W, Mo) Ceramics by modified Becke-Johnson Potential*, *Optical Materials* 58 (2016) 466-475
2. A. Khan, **Zahid Ali**, I. Khan, I. Ahmad, S.J. Asadabadi, "First Principles Studies of the Ternary Palladates  $\text{CaPd}_3\text{O}_4$  and  $\text{SrPd}_3\text{O}_4$ ", *Bulletin of Materials Science* (2016) Accepted
3. A. Abdullah, I. Khan, **Zahid Ali**, I. Ahmad "Thermoelectric studies of IV-VI semiconductors for renewable energy resources" *Materials Science in Semiconductor Processing* 48 (2016) 85-94
4. I. Khan, S. Khan, **Zahid Ali**, H.A.R. Aliabad, I. Ahmad, J. Iqbal "The influence of oxygen substitution on the optoelectronic properties of ZnTe" *J. Chemistry*, 2016 (2016) 1–8
5. S. Ahmad, I. Khan, **Zahid Ali**, A.A. Khan, R. Ahmad, I. Ahmad, H.R.A. Aliabad "First principle studies of pure and fluorine substituted alanine" *Int. J. Mod. Phys. B*, 30 (2016) 1650079 (1-13)
6. **Zahid Ali**, A. Sattar, I. Ahmad, S.J. Asadabadi "Theoretical studies of the osmium based perovskites  $\text{AOsO}_3$  (A = Ca, Sr and Ba)" *J. Phys. Chem. Solids* 86 (2015) 114–121
7. **Zahid Ali**, I. Khan, I. Ahmad, M.S. Khan, S.J. Asadabadi "Theoretical Studies of the Paramagnetic Perovskites  $\text{MTaO}_3$  (M= Ca, Sr and Ba)" *Materials Chemistry and Physics* 162 (2015) 308-315

8. I. Khan, F. Subhan, I. Ahmad, **Zahid Ali** “Structural and optoelectronic properties of Mg substituted ZTe ( $Z = \text{Zn, Cd and Hg}$ )” *J. Phys. Chem. Solids* 83 (2015) 75–84
9. R. Zeb, **Zahid Ali**, I. Ahmad, I. Khan “Structural and Magnetic Properties of  $\text{TlTF}_3$  ( $T = \text{Fe, Co and Ni}$ ) by Hybrid Functional Theory” *J. Magnetism and Magnetic Materials* 388 (2015) 142-149
10. **Zahid Ali**, B. Khan, I. Ahmad, I. Khan “Magneto-electronic studies of the Inverse Perovskite  $(\text{EuO}_3)\text{In}$ ” *J. Magnetism and Magnetic Materials* 38 (2015) 34-40
11. S. Sadiq, **Zahid Ali**, I. Khan, I. Ahmad, G. Rehman, M. Sadiq, N. U. Rehman "Structural, Mechanical and Magneto-Electronic Properties of the Ternary Sodium Palladium and Platinum Oxides" *Z. Naturforsch.* 70(10) (2015) 815–822
12. R. Iqbal, I. Khan, **Zahid Ali**, I. Ahmad, “Density Functional studies of Magneto-optic properties of  $\text{CdCoS}$ ” *J. Magnetism and Magnetic Materials* 351 (2014) 60-64
13. **Zahid Ali**, I. Ahmad, M. Shafiq, I. Khan “Magneto-electronic studies of the cubic anti-perovskites  $\text{NiNMn}_3$  and  $\text{ZnNMn}_3$ , *Comput. Mater. Sci.* 81 (2014) 141-145
14. I. Khan, H. A. Rahnamaye Aliabad, W. Ahmad, **Zahid Ali**, I. Ahmad “First principle optoelectronic studies of visible light sensitive CZT” *Superlattices and Microstructures* 63 (2013) 91–99 [
15. **Zahid Ali**, I. Khan, I. Ahmad, S. Jalali Asadabadi, S. Naeem, H.R.Aliabad, D. Zhang, “Comparison of the electronic band profiles and magneto-optic properties of cubic and orthorhombic  $\text{SrTbO}_3$ ” *Physica B* 423 (2013)16–20
16. I. Khan, I. Ahmad, H. A. Rahnamaye Aliabad, S. Jalali Asadabadi, **Zahid Ali**, M. Maqbool “Conversion of optically isotropic to anisotropic  $\text{CdS}_x\text{Se}_{1-x}$  ( $0 \leq x \leq 1$ ) alloy with the substitution of S” *Comput. Mater. Sci.* 77 (2013) 145–152

17. **Zahid Ali**, I. Ahmad, S. Ali, I. Khan “Structural and optoelectronic properties of the zinc titanate perovskite and spinel by modified Becke-Johnson potential” *Physica B* 420 (2013) 54-57
18. **Zahid Ali**, I. Ahmad, B. Khan. I. Khan “Magneto-electronic and robust studies of the cubic perovskite  $\text{CaFeO}_3$ ” *Chin. Phys. Lett.* 30, (2013) 047504
19. **Zahid Ali**, I. Ahmad, “Band profile comparison of the cubic perovskites  $\text{CaCoO}_3$  and  $\text{SrCoO}_3$ ” *J. Electronic materials.*42, (2013) 438-444
20. **Zahid Ali**, I. Ahmad, A. H. Reshak “GGA+U studies of the cubic perovskites  $\text{BaMO}_3$  ( $M= \text{Pr, Th and U}$ )” *Physica B* 410, ( 2013) 217–221
21. **Zahid Ali**, I. Ahmad, S.J. Asadabadi “Comparison of band profile and magnetic properties of the different phases of  $\text{BaTbO}_3$ ” *Comput. Mater. Sci.* 67 (2013) 151-155
22. **Zahid Ali**, I. Ahmad, I. Khan B. Amin “Electronic structure of cubic  $\text{SnTaO}_3$ ” *Intermetallics* 31 (2012) 287–291
23. **Zahid Ali**, I. Ahmad, B. Amin, M. Maqbool, G. Murtaza, I. Khan, M. J. Akhtar, F. Ghafor. “Theoretical studies of structural and magnetic properties of cubic perovskites  $\text{PrCoO}_3$  and  $\text{NdCoO}_3$ ” *Physica B* 406 (2011) 3800-3804
24. I. Khan, I. Ahmad, B. Amin, G. Murtaza, **Zahid Ali** “Bandgap engineering of  $\text{Cd}_{1-x}\text{Sr}_x\text{O}$ ” *Physica B* 406 (2011) 2509-2514
25. G. Murtaza, I. Ahmad, B. Amin, A. Afaq, M. Maqbool, J. Maqsod, I. Khan, **Zahid Ali**, Investigation of structural and optoelectronic properties of  $\text{BaThO}_3$ , *Optical Materials* 33 (2011) 553-557