

## **Curriculum Vitae**

### **DR. ZAHID ALI**

Assistant Professor, Department of Physics  
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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, 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): Govt. Degree College Badh Bare, Peshawar, KP, Pakistan

### **Administrative Experiences**

- Member of Graduate Studies Committee, Department of Physics, University of Malakand from Feb. 2, 2017 to Present
- Member Board of Studies of Physics, Abbotabad University of Science and Technology Abbotabad, from Sep. 2016 onward
- Semester coordinator in the Department of Physics, University of Malakand from Dec. 18, 2014 to Dec. 18, 2017.

### **Expertise**

- Organizing National/ International Conferences/ Workshops, Curriculum Development, Students Management, Financial Management etc.

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

- Organizer of the Workshop on Materials Modeling and Simulations held at AUST, Abbottabad on March 1<sup>st</sup> and 2<sup>nd</sup>, 2017
- 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.
- 27<sup>th</sup> National and 15<sup>th</sup> International Chemistry Conference held at University of Malakand (Pakistan) Aug. 22 to 25, 2016.

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

- 1<sup>st</sup> National conference on Advances in Physics held at Department of Physics, University of Malakand (Pakistan) Nov. 06 to 07, 2017.
- 1<sup>st</sup> National conference on Emerging Trends in Materials Science held at Department of Physics, Abbotabad University of Science and Technology Abbotabad (Pakistan) Oct, 05 to 07, 2017.

- 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 Applications” 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 by-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

#### **Ph.D Students Under Supervision**

1. Mr. Shahid Mehmood
2. Mr. Rahman Zada
3. Mr. Noor Ullah
4. Mr. Murad

### **Ph.D Students Under Co-Supervision**

1. Amin Khan “Physical Properties of  $APd_3O_4$  (A= Ca, Sr, Cd and Tl) Types Palladates; An ab-initio Study”

### **M. Phil Students Supervised**

1. Mr. Abdul Sattar “DFT Studies of  $AOsO_3$  (A=Ca, Sr and Ba) Perovskites”
2. Mr. Rahm Zeb “Structural, Elastic, Electronic and Magnetic Studies of  $TiTF_3$  (T=Fe, Co and Ni)”
3. Mr. Mazhar Rahman “ab-initio Studies of Double Perovskites  $LiMMoO_6$  (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  $Al_{13}Fe_4$ ”
5. Mr. Muhammad Sadiq “First principle studies of Mg-rich intermetallic  $NdNiMg_5$ ”
6. Mr. Noor Ullah “Theoretical studies of  $Y_2M_2O_7$  (M = Ti, V and Nb) pyrochlores”
7. Mr. Muhammad Ayoub “Variation in the physical properties of  $La_{0.5}Ba_{0.5}CoO_3$ ,  $LaBaCo_2O_{5.5}$  and  $LaBaCo_2O_6$ ”
8. Mr. Shahid Mehmood “Theoretical studies of  $SrFe_xCo_{1-x}O_3$  (X= 0.25, 0.5, 0.75 and 1)”
9. Mr. Rahman Zada, “Hybrid DFT Studies of Inverse Perovskites  $(Ln_3N)Sn$  (Ln = La, Ce, Pr, Nd and Sm)”
10. Mr. Abdul Wakil, “Investigation of the Electronic Structure and Magnetic Properties of the Perovskites  $NdTMO_3$  (TM= Cr, Mn, Fe and Co)”
11. Mr. Asim Mehmood, “First Principles Studies of the Magneto-electronic Properties of the Pyrochlore  $Dy_2Ti_2O_7$  and  $Ho_2Ti_2O_7$ ”
12. Ms. Somia Hayat, “DFT Studies of the Perovskite Molybdates  $AMoO_3$  (A = Ca, Sr and Ba)”
13. Mr. Farman Ullah “Electronic Structure and Magnetic Properties of the Perovskites  $ABO_3$  (A = Sr, Ba and B = Pu, Am)”
14. Mr. Ahmad Shah “Electronic Structure, Mechanical and Magnetic Properties of the Quaternary Perovskites  $CaA_3V_4O_{12}$  (A = Mn, Fe, Co, Ni and Cu)”

15. Ms. Samreen Gul “Electronic Structure and Magnetic Properties of the Rare-Earth Perovskite  $\text{LnMn}_3\text{V}_4\text{O}_{12}$  (Ln=La, Nd and Gd)”
17. Mr. Muhammad Idrees “Mechanical Analysis and Magnetic Ordering of the Binary Intermetallic Compounds  $\text{RFe}_2$  (R = La, Ce, Pr and Nd)”
18. Mr. Layaq Akbar

### **Courses Thought:**

#### **Graduate Level:**

- (i) Magnetism in Condensed Matter
- (ii) Mathematical Methods for Theoretical Physics
- (iii) Materials Science-I & II
- (iv) Classical Mechanics
- (v) Statistical Mechanics
- (vi) Theory of Condensed Matter

#### **Undergraduate Level:**

- (i) Solid State Physics (I & II)
- (ii) Thermal and Statistical Physics (I & II)
- (iii) Heat and Thermodynamics
- (iv) Electricity and Magnetism
- (v) Mechanics

### **Publications: [Impact factor]**

1. I. Ullah, S. Mehmood, **Zahid Ali**, I. Khan, I. Ahmad, G. Rehaman “Theoretical Studies of the Electronic Structure and Magnetic Properties of Aluminum-Rich Intermetallic Alloy  $\text{Al}_{13}\text{Fe}_4$ ” *Int. J. Mod. Phys. B* (2018) Accepted
2. S. Ahmad, R. Ahmad, S. J. Asadabadi, **Zahid Ali**, I. Ahmad “First principle studies of structural, magnetic and elastic properties of orthorhombic rare-earth diaurides intermetallics  $\text{RAu}_2$  (R=La, Ce, Pr and Eu)” *Mater. Chem. Phys.* **212** (2018) 44-50

3. A. Khan, **Zahid Ali**, I. Khan, I. Ahmad “Electronic Structure, Mechanical and Thermoelectric Properties of the Ternary Palladates CdPd<sub>3</sub>O<sub>4</sub> and TIPd<sub>3</sub>O<sub>4</sub>: A First Principles Study” J. Electronic Materials **47**(3) (2018) 1871-1880
4. N. Ullah, **Zahid Ali**, I. Khan, G. Rehman, I. Ahmad “Structural, Mechanical and Optoelectronic Properties of the Pyrochlores Y<sub>2</sub>M<sub>2</sub>O<sub>7</sub> (M = Ti, V and Nb): A First Principles Study” J. Electronic Materials **46** (7), (2017) 4640-4648
5. R. Iqbal, **Zahid Ali**, I. Ahmad, S.J. Asadabadi “Electron Correlation and Spin-Orbit Coupling Effects in Scandium Intermetallic Compounds ScTM (TM= Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au)” Int. J. Mod. Phys. B **31** (2017) 1750263 (17 pages)
6. S. Mehmood, **Zahid Ali**, I.Khan, I.Ahmad “Effects of Cobalt Substitution on the Physical Properties of the Perovskite Strontium Ferrite” Materials Chemistry and Physics **196**, (2017) 222-228
7. I. Khan, **Zahid Ali**, N. Shahzad, I. Ahmad, S.J. Asadabadi “First principle studies of the optoelectronic properties of ASnF<sub>3</sub> (A = Na, K, Rb and Cs)” Int. J. Modern Physics B **31**, (2017) 1750148
8. S. Ahmad, R. Ahmad, **Zahid Ali**, I. Ahmad, S.J. Asadabadi “First principle studies of electronic and magnetic properties of Lanthanide-Gold (RAu) binary Intermetallics” J. Magnetism and Magnetic Materials 422 (2017) 458–463
9. **Zahid Ali**, I. Khan, M. Rehman, I. Ahmad, R. Ahmad, Electronic Structure of the LiAA'O<sub>6</sub> (A = Nb, Ta, and A' = W, Mo) Ceramics by modified Becke-Johnson Potential, Optical Materials 58 (2016) 466-475 [**2.20**]

10. 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 39 (7) (2016) 1861–1870 [1.02]
11. A. Abdullal, 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 [1.95]
12. 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 [0.77]
13. 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) [0.94]
14. **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[1.85]
15. **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 [2.24]
16. I. Khan, F. Subhan, I. Ahmad, **Zahid Ali** "Structural and optoelectronic properties of Mg substituted ZTe (Z = Zn, Cd and Hg) J. Phys. Chem. Solids 83 (2015) 75–84 [1.85]
17. R. Zeb, **Zahid Ali**, I. Ahmad, I. Khan "Structural and Magnetic Properties of  $\text{TlTF}_3$  (T = Fe, Co and Ni) by Hybrid Functional Theory" J. Magnetism and Magnetic Materials 388 (2015) 142-149 [1.97]

18. **Zahid Ali**, B. Khan, I. Ahmad, I. Khan “Magneto-electronic studies of the Inverse Perovskite (EuO<sub>3</sub>)In” J. Magnetism and Magnetic Materials 38 (2015) 34-40 [**1.97**]
19. 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 [**0.85**]
20. R. Iqbal, I. Khan, **Zahid Ali**, I. Ahmad, “Density Functional studies of Magneto-optic properties of CdCoS” J. Magnetism and Magnetic Materials 351 (2014) 60-64 [**1.97**]
21. **Zahid Ali**, I. Ahmad, M. Shafiq, I. Khan “Magneto-electronic studies of the cubic anti-perovskites NiNMn<sub>3</sub> and ZnNMn<sub>3</sub>, Comput. Mater. Sci. 81 (2014) 141-145 [**2.13**]
22. 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 [**2.10**]
23. **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 SrTbO<sub>3</sub>” Physica B 423 (2013)16–20 [**1.32**]
24. I. Khan, I. Ahmad, H. A. Rahnamaye Aliabad, S. Jalali Asadabadi, **Zahid Ali**, M. Maqbool “Conversion of optically isotropic to anisotropic CdS<sub>x</sub>Se<sub>1-x</sub> (0 ≤ x ≤ 1) alloy with the substitution of S” Comput. Mater. Sci. 77 (2013) 145–152 [**2.13**]
25. **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 [**1.32**]
26. **Zahid Ali**, I. Ahmad, B. Khan. I. Khan “Magneto-electronic and robust studies of the cubic perovskite CaFeO<sub>3</sub>” Chin. Phys. Lett. 30, (2013) 047504 [**0.94**]



27. **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 [**1.80**]
28. **Zahid Ali**, I. Ahmad, A. H. Reshak “GGA+U studies of the cubic perovskites  $\text{BaMO}_3$  (M= Pr, Th and U)” Physica B 410, ( 2013) 217–221 [**1.32**]
29. **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 [**2.13**]
30. **Zahid Ali**, I. Ahmad, I. Khan B. Amin “Electronic structure of cubic  $\text{SnTaO}_3$ ” Intermetallics 31 (2012) 287–291 [**2.13**]
31. **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 [**1.32**]
32. 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 [**1.32**]
33. 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 [**1.98**]

**Papers under Review:**

1. **Zahid Ali**, I. Khan, *Iftikhar Ahmad*, “First Principle Studies of the Molybdates  $\text{AMoO}_3$  (A = Ca, Sr and Ba)” J. Materials Science

### Academics References:

- Prof. Dr. Iftikhar Ahmad  
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