

CURRICULUM VITAE

AFAQ AHMAD

Professor (Tenured)

Centre of Excellence in Solid State Physics

University of the Punjab Lahore

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I did PhD (Theoretical Physics) in 2007 working under the supervision of Prof. Dr. Du Ming Li, at Institute of Theoretical Physics (ITP) Beijing, China under the Higher Education Commission (HEC) Basic-sciences scholarship program. During PhD study, I succeeded in formulating the Theoretical Imaging Method (TIM) and Two-center Model, new theoretical tools to understand negative ions photo-detachment near different surfaces. After PhD, I joined the Department of Physics, COMSATS University Islamabad (CUI) Lahore Campus in 2007 as an Assistant Professor. Subsequently, as an Assistant Professor on TTS, I joined the Centre of Excellence in Solid State Physics (CSSP), University of the Punjab in 2009. In 2014, the Board of Governor Meeting, in view of my extraordinary performance at the Centre of Excellence in Solid State Physics, promoted me as an Associate Professor. In 2021, the Board of Governor (BOG) Meeting at the Centre of Excellence in Solid State Physics promoted me to the next higher rank as Professor (Tenured). Presently, I am running a material simulation research lab where the structural, optical, magnetic, elastic, mechanical, vibrational, and thermodynamic properties of different crystals are being investigated. Also heading a theoretical group in ion-photon interaction near different surfaces and collaborating in photonic crystals and quantum optics.

119 research publications, one book, 49 conference presentations, 109 M. Phil. theses and 14 PhD theses were produced by me during the period from 2006-2025 working on the following research fields:

1. Atomic and Molecular Physics (Ion-Photon Interaction)
2. Material Simulation (Density Functional Theory Calculations)
3. Photonic Crystals
4. Theory of Thin Films

EDUCATIONAL QUALIFICATION:

1. Ph. D. (Theoretical Physics) (2007)

Institute of Theoretical Physics (ITP), Chinese Academy of Sciences Beijing China

Thesis Title: Interferences in the Photo-detachment of Negative Ion Systems

2. M. Phil. (Solid State Physics) (1995)

COE in Solid State Physics, University of the Punjab Lahore

Thesis Title: Reductive perturbation Methods and their Applications in the study of Non- linear Wave Propagation

3. M. Sc. (Physics) (1991)

Quid-e-Azam University Islamabad

4. B. Sc. (Physics, Math A & B) (1989)

Govt. Islamia College Civil Lines Lahore

5. F. Sc. (Pre-Engineering) (1987)

Govt. Islamia Post Graduate College Kasur

6. Metric (Science) (1985)

Govt. Model High School Kasur

WORK EXPERIENCE:

I have been working as a lecturer in the Punjab education department in various colleges since from 1995 to 2004. After PhD, I worked as Assistant Professor in the Department of physics, COMSATS University Islamabad (CUI) Lahore campus from 2007 to 2009. Subsequently, I worked as Assistant Professor (2009-2014) and then Associate Professor (2014-2021) at the Center of Excellence in Solid State Physics, University of the Punjab, Lahore, where onward from 2021, I am working as a Professor. The detailed of my work experience is as under:

1. Lecturer in Physics (1995-1996)

Govt. Post Graduate College Chakwal, Pakistan

2. Lecturer in Physics (1996-1998)

Govt. Degree College JSK Sheikhpura, Pakistan

3. Lecturer in Physics (1998-2001)

Govt. MAO College Lahore, Pakistan

4. Lecturer in Physics (2001-2004)

Govt. Islamia College Kasur, Pakistan

5. HEC PhD Scholar (2004-2007)

Institute of Theoretical Physics (ITP), CAS, Beijing China

6. Assistant Professor in Physics (2007-2009)

COMSATS University Islamabad, Lahore Campus, Pakistan

7. Assistant Professor (2009-2014)

Center of Excellence (COE) in Solid State Physics, University of the Punjab Lahore, Pakistan

8. Associate Professor (2014-2021)

Center of Excellence (COE) in Solid State Physics, University of the Punjab Lahore, Pakistan

9. Tenured Professor (2021 to date)

Center of Excellence (COE) in Solid State Physics, University of the Punjab Lahore, Pakistan

AWARDS:

- 1.** Merit Scholarship in B. Sc. (1987-1989)
- 2.** Merit Scholarship in M. Sc. (1989-1991)
- 3.** Runner-up Position (Badminton) at QAU Islamabad (1989-1991)
- 4.** Infaq Scholarship in M. Phil. (1993-1995)
- 5.** HEC Scholarship in Ph. D. (2004-2007)
- 6.** Research Productivity Award 2011
- 7.** Performance-based Honorarium & increment 2012
- 8.** Performance-based Honorarium & increment 2013
- 9.** Research Productivity Award 2012
- 10.** Research Productivity Award 2013
- 11.** Performance-based increment 2014
- 12.** Performance-based increment 2015
- 13.** Performance-based Honorarium & increment 2017
- 14.** Performance-based Honorarium & increment 2018
- 15.** Performance-based Honorarium & increment 2019
- 16.** Performance-based Honorarium & increment 2020
- 17.** Performance-based increment 2021
- 18.** Performance-based Honorarium & increment 2022
- 19.** Performance-based Honorarium & increment 2023
- 20.** Performance-based Honorarium & increment 2024
- 21.** Performance-based Honorarium & increment 2025

COURSES TAUGHT TO MPhil AND PHD CLASSES:

1. Semiconductor Theory
2. Defects in Solids
3. Lattice Dynamics
4. Optical Properties of Solids
5. Nanomaterials: A Theoretical Approach

MEMBERSHIP

1. Pakistan Institute of Physics (PIP)
2. Khwarzimid Science Society (KSS)
3. Department Promotion Committee (DPC), COE in Solid State Physics, University of the Punjab Lahore
4. Department Technical Review Committee (DTRC), COE in Solid State Physics, University of the Punjab Lahore
5. Department Technical Review Committee (DTRC), Department of Physics, University of the Punjab Lahore
6. Department Technical Review Committee (DTRC), Center of High Energy Physics, University of the Punjab Lahore
7. Board of Studies (BOS), Department of Physics, The University of Azad Jammu & Kashmir Muzaffarabad
8. Department Technical Review Committee (DTRC), Department of Physics, The University of Azad Jammu & Kashmir Muzaffarabad
9. Board of Studies (BOS), Department of Physics, Virtual University Lahore
10. Academic Council, Khawja Fareed University of Engineering & Information Technology, Rahim Yar Khan

RESEARCH PUBLICATIONS [114]:

2006.....(**IF=2.9**)

1. Interferences in Photo-detachment of a Negative Molecular Ion

A Afaq and M. L. Du, Commun. Theor. Phys., **46** (2006) 119 (IF=2.9)

2007.....(**IF=1**

.5)

2. A theoretical imaging method for the photo-detachment of H⁻ near a reflecting surface

A Afaq and M. L. Du, J. Phys. B: At. Mol. Opt. Phys., **40** (2007) 1309 (IF=1.5)

2008.....(**IF=3.4**)

3. Interferences in Photo-detachment of a Negative Molecular Ion Model

A Afaq and M. L. Du, Commun. Theor. Phys., **50** (2008) 1401 (IF=2.9)

4. A study of FBG sensor and electrical strain gauge for strain measurements

B. A. Tahir, J. Ali Saktioto, M. Fadhali, R. A. Rahman, **A Afaq**, J. Optoelectronics and Advanced Materials, **10** (2008) 2564 (IF=0.5)

2009..... (**IF=8.7**)

5. Effect of Laser and Mechanical Parameters on Strength of Fiber Bragg Gratings

Bashir Ahmed Tahir, Abdul Rashid , M. Asif , **A. Afaq**, Jalil Ali and RoslyAbdul Rahman, International Journal of Modern Physics B, **23** (2009) 77 (IF=2.3)

6. Interferences in the Photo-detachment of a Tri-atomic negative molecular ion

A Afaq, M. A. Ahmad, A. Rashid, Iftikhar Ahmad, B. A. Tahir, and TahirHussain Applied Physics Letters **94** (2009) 041125 (IF=3.6)

7. Oscillations in the Photo-detachment cross sections of a two-center system

A Afaq and M. L. Du, J. Phys. B: At. Mol. Opt. Phys., **42** (2009) 105101 (IF=2.3)

8. An investigation of linearity and sensitivity of Fiber Bragg Grating sensors

B. A. Tahir, J. Ali, A. Rahman, **A Afaq**, Journal of Optoelectronics and Advanced Materials, **11** (2009) 1692 (IF=0.5)

2010.....(**IF=**)

9. Generalized gradient calculations of structural, electronic and optical properties of $Mg_xCd_{1-x}O$ oxides
Bin Amin, Iftikhar Ahmad, Muhammad Maqbool, NazmaIkram, Yasir Saeed, **A Afaq**, Sunila Arif, Journal of Alloys and Compound **493** (2010) 212
10. Oscillations in the photo-detachment of a linear tri-atomic negative ion
A Afaq, M. Hanif and Iftikhar Ahmad arxiv: 1001.4183v1 (2010)
- 2011**.....(IF=)
11. Classification of partially reflecting surfaces using Photo-detached electron spectrum
A. Afaq and Iftikhar Ahmad, Int. J. of Quantum Chem. **111** (2011) 4067
12. Investigation of spherical effects on the photodetached electron-spectra
M. Haneef, Iftikhar Ahmad, **A. Afaq**, A. Rahman, J. Phys. B: At. Mol. Opt. Phys. **44** (2011) 195004
13. Interferences in the photodetached-electron spectra from a linear tetra-atomic negative ion
A Rehman, Iftikhar Ahmad, **A. Afaq**, M. Haneef, Chin. Phys. Lett **28** (2011) 063301
14. Investigation of a linear tetra-atomic negative ion by photodetached-electron spectra
A.Rehman, Iftikhar Ahmad, **A. Afaq**, M. Haneef, H. J. Zhao, Chin. Phys. Lett., **28**(8) (2011) 083301
15. Investigation of structural and optoelectronic properties of BaThO3
G. Murtaza, Iftikhar Ahmad, B. Amin, **A. Afaq**, M. Maqbool, J. Maqssod, I. Khan and M. Zahid, Optical Materials **33** (2011) 553-557
16. Linear and non-linear optical response of $Mg_xZn_{1-x}O$: A Density Functional study
G. Murtaza, Iftikhar Ahmad, B. Amin, **A. Afaq**, F. Ghafoor, A. Benamrani, Physica B: condense matter, **406** (2011) 2632
17. First principle study of cubic perovskites: $AgTF_3$ (T=Mg, Zn)
G. Murtaza, G. Sadique , H. A. Rahnamaye Aliabad, M. N. Khalid , S. Naeem, **A. Afaq**, B. Amin, Iftikhar Ahmad, Physica B: Condensed Matter **406** (2011) 4584
18. Structural and Optoelectronic Properties of Cubic $CsPbF_3$ for Novel Applications
G. Murtaza, Iftikhar Ahmad, M. Maqbool, H. A. Rahnamaye Aliabad, **A. Afaq** Chin. Phys. Lett. **28**(11), 117803 (2011)

19. Effect of Sensor Gauge Length on Strain Sensitivity of Fiber Bragg Grating System
B A Tahir, A. Saeed, **Afaq Ahmed**, S. M. Zafar Iqbal, Rashid Ahmed, M. Gul Baha Ashiq, Hewa Yaseen Abdullah, and Rosly Abdul Rahman, Chinese journal of Physics, **49** (2011) 1035

2012.....(IF=)

20. Cutting of Nonmetallic Materials Using Nd: YAG Laser Beam
Bashir Ahmed Tahir, Rashid Ahmed, M. G. B. Ashiq, Rosly Abdul Rahman, **A Afaq** and M. A. Saeed, Chinese Physics B, **21** (2012) 044201
21. Photo-detachment of H^- near a Hard Spherical Surface
M. Haneef, Iftikhar Ahmad, **A. Afaq**, A. Rahman, Chin. Phys. Lett., **29** (2012) 013202
22. Structural, electronic and optical properties of $Ca_xCd_{1-x}O$ and its conversion from semimetal to wide band gap semiconductor
G. Murtaza, B. Amin, S. Arif, M. Maqbool, I. Ahmad and **A. Afaq**, S. Nisar, M. Imran, M. Hanif, Computational Materials Science, **58** (2012) 71
23. Photo-detachment of a Homo-Nuclear Linear Tetra-Atomic Negative Molecular Ion
A. Rahman, Iftikhar Ahmad, **A. Afaq**, H. J. Zhao, Chin. Phys. Lett., **29** (2012) 043301
24. Transition from optically inactive to active Mg-Chalcogenides: A first principle study
Imad Khan, **A. Afaq**, H. A. Rahnamaye Aliabad, and Iftikhar Ahmad, Computational Materials Science, **61** (2012) 278
25. A Comprehensive DFT Study of Zinc Oxide in Different Phases
Bakhtiar Ul Haq, **A. Afaq**, R. Ahmed and S. Naseem Int. J. Mod. Phys. C, **23** (2012) 1250043
26. Structural, Electronic and Magnetic Properties of Co-Doped ZnO
Bakhtiar Ul Haq, **A. Afaq**, R. Ahmed and S. Naseem, Chinese physics B **21** (2012) 097101
27. Structural, Electronic and Optical Properties of MgS_xSe_{1-x} , MgS_xTe_{1-x} and $MgSe_xTe_{1-x}$ ($0 < x < 1$) alloys From First Principles
A. Sajid, S. M. Alay-e-Abbas, **A. Afaq** and A. Shaukat, Int. J. Mod. Phy. B, **26** (2012)

1250098

28. Classical Limit in the Photo-detachment of a Diatomic Anion: A Two Center Model Approach

Sadia Ashiq, **Afaq Ahmad**, Sci. Int. (Lahore), **24** (2012) 113

29. Photo-detached Electronic Wave Function of Hydrogen Halide Anions

Ayesha Amjad, **Afaq Ahmad**, Maryam Nawaz, Sadia Ashiq, Sci. Int. (Lahore), **24** (2012) 337

2013.....(IF=)

30. Shift of indirect to direct band gap in going from K to Cs in $MCaF_3$ (M=K, Rb, Cs)

G. Murtaza, Iftikhar Ahmad, **A. Afaq**, Solid State Sciences, **16** (2013) 152

31. Electron Flux Distributions in Photodetachment of HF^- near an interface: Theoretical Imaging method Study

Maryam Nawaz Awan and **A. Afaq**, Chinese Physics B, **22** (2013) 013205

32. Photo-detachment of H^-

Tyyiba Fiyazi, **Afaq Ahmad**, Int. Sci. (Lahore), **25** (2013) 71

33. First Principle study of Electronic and Optical Properties of Magnesium based Chalcogenides

A.Sajjid, **A. Afaq** and G. Murtaza, Chinese Journal of Physics, **51** (2013) 328

34. Electronic structure engineering of ZnO with the modified Becke-Johnson exchange versus the classical correlation potential approaches

Bakhtiar Ul Haq, R. Ahmed, Souraya Goumri-Said, A. Shaari and A. Afaq, Phase Transitions, **86** (2013) 1167

35. Dissociation Distance of H_2^- Molecule: Two-center Model Study

Sadia . A. **Afaq**, A. Shahzad. A. Muhammad Masood, Int Sci. (Lahore), **25** (2013) 693

2014.....(IF=)

36. A Study of Cr doping on the Structural and Electronic Properties of ZnO: A First Principles Study

BAKHTIAR UL HAQ, R. AHMED, A. SHAARI, **A. AFAQ** & R. HUSSAIN, Sains Malaysiana, **43** (2014) 813

37. Interferences in Photo-detached Electron Spectra from a non-collinear triatomic anion

- A.Afaq**, K. Farooq, M. A. Khan, X. X. Yi,
Chinese Physics B, **23** (2014) 103304
38. Photo-detachment of a non-collinear triatomic anion
A.Afaq, K. Farooq, Brazilian J. Phys. **44** (2014) 609
39. First Principles Band-gap Calculations of 3d Transition Metals-added Rock-salt ZnO
M. Ashraf, **A. Afaq**, Research & Reviews: Journal of Physics, **3** (2014) 1
- 2015**.....(IF=)
40. First-principles Investigations of Mn doped zinc-blende ZnO based Magnetic Semiconductors: Materials for Spintronic applications
Bakhtiar Ul Haq, R. Ahmed, A. Shaari, **A. Afaq**, B. A. Tahir, R. Khenata, Materials Science in Semiconductor Processing, **29** (2015) 256
41. First Principles Study of Scandium Nitride and Yttrium Nitride Alloy System: prospective material for optoelectronics
Bakhtiar Ul Haq, **A. Afaq**, Galila Abdellatif, R. Ahmed, S. Naseem, Rabah Khenata Superlattices and Microstructures, **8** (2015) 524
42. Photo-detachment of H⁻ near a hard elastic wall with arbitrary laser Polarization
AzmatIqbal, **A. Afaq**, Chinese Physics B, **24** (2015) 083201
43. Photodetachment of H⁻ Near Inelastic Surfaces: Arbitrary Laser Polarization Direction
Azmat Iqbal, **A. Afaq**, R. J. Amjad, Int. j. Quantum Chem., **15** (2015) 1526
44. Structural, electronic and elastic properties of the cubic CaTiO₃ under pressure: A DFT study
Saad Tariq, **Afaq Ahmed**, SaherSaad, Samar Tariq, AIP, Advances, **5** (2015) 077111
45. Putting DFT to the Trial: First principles pressure dependent analysis on optical properties of cubic perovskite SrZrO₃
Ghazanfar Nazir, **Afaq Ahmad**, Muhammad Farooq Khan, Saad Tariq, Computational Condensed Matter, **4**, 32 (2015)
46. Theoretical photo detachment microscopy of H⁻ ion near an interface using theoretical imaging method
Maryam Nawaz Awan, Afaq Ahmad, Mujahid Kamran, Material Today: Proceedings, **2** (2015) 5136

47. First principles band-gap calculations of 3d transition metals added ZnO
 Muhammad Ashraf, Afaq Ahmad, *Material Today: Proceedings* **2** (2015) 5128
- 2016.....(IF=)**
48. Photodetachment spectrum of hydrogen negative ion near a spherical surface **A. Afaq**, A. Iqbal, A. Iftikhar, and M. Asif, *Canadian J. Phys.*, **94** (2016) 26
49. Photodetachment Spectrum of Hydrogen Negative Ion Near a Partially Reflecting Spherical Surface
A. Afaq, AzmatIqbal, Amin Ur Rahman, Naveed Khan, Fazal-e-Aleem, M. Mushraf Ansari, *Braz. J. Phys.* **46** (2016) 489
50. Pressure-Dependent Structural and Optical Properties of CdSe
 Ali Asad, **Afaq Ahmad**
Research & Reviews: Journal of Physics, **5** (2016) 1
51. Structural and Optical Properties of ZnSe Under Pressure
 Ali Asad, **Afaq Ahmad**
Research & Reviews: Journal of Physics, **5** (2016) 6
- 2017.....(IF=)**
52. Thermodynamic properties of ZnSe under pressure and with variation in temperature
 Najm Ul Aarifeen and **A Afaq**, *Chines Physics B*, **26** (2017) 093105
53. Gain-assisted superluminal propagation and rotatory drag of photon and surface Plasmon polaritons
 Naveed Khan, Bakht Amin Bacha, Azmat Iqbal, Amin Ur Rahman, and **A. Afaq**, *Physical Review A*, **96** (2017) 013848
54. Effects of temperature and pressure on thermodynamic properties of Cd_{0.50}Zn_{0.50}Se alloy
 Najm Ul Aarifeen and **A Afaq**, *Mater. Res. Express*, **4** (2017) 095901
55. Photon drag enhancement by a slow-light moving medium via electromagnetically-induced transparency amplification
 Azmat Iqbal, Naveed Khan, Bakht Amin Bacha, Amin Ur Rahman, **Afaq Ahmad**
Physics Letters A, **381** (2017) 3134
56. Effects of temperature and pressure on thermodynamic properties of Cd_{0.25}Zn_{0.75}Se alloy

Najm Ul Aarifeen and **A Afaq**, Chines Physics B, **26** (2017) 123101

57. First-principles study of structural, electronic, magnetic and thermoelectric properties of the cubic mono-pnictides of thorium ThPn ($Pn = Sb$ and Bi)

Muhammad Siddique, Amin Ur Rahman¹, Bakhtiar Ul Haq, Azmat Iqbal, **Afaq Ahmad**, Iftikhar Ahmad, 432, **13** (2107) 111

58. Erratum: Gain-assisted superluminal propagation and rotary drag of photon and Surface plasmon polaritons [Phys. Rev. A **96** (2017) 013848

Naveed Khan, Bakht Amin Bacha, Azmat Iqbal, Amin Ur Rahman, and **A. Afaq** Physical Review A, **96** (2017) 049906(E)

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59. DFT study on thermo-elastic properties of Ru_2FeZ ($Z=Si, Ge, Sn$) Heusler alloys

Aneeza Iftikhar, **Afaq Ahmad**, Iftikhar Ahmad, Muhammad Rizwan, International Journal of Modern Physics B, **32** (2018) 1850045

60. Under Pressure DFT Investigations on Optical and Electronic Properties of $PbZrO_3$

G. Nazir, Saad Tariq, **A. Afaq**, Q. Mahmood, S. Saad, A. Mahmood and Samar Tariq, ACTA PHYSICA POLONICA A, **133** (2018) 105

61. Lattice dynamics of Ru_2FeX ($X = Si, Ge$) Full Heusler alloys

M. Rizwan, **A. Afaq**, A. Aneeza, Physica B-Condensed Matter, **537** (2018) 225

62. Electronic and magnetic properties of $BaUO_3$ by modified Becke-Johnson (mBJ) functional

Ghulam Mustafa, Najm ul Aarifeen, **Ahmad Afaq** and Muhammad Asif, Modern Physics Letters B, **32** (2018) 1850164

63. Theoretical study of thermodynamic properties for $SmAlO_3$ under the effects of pressure and temperature

Ghulam Mustafa, **Ahmad Afaq**, Najm Ul Aarifeen, Muhammad Asif, Jamil Ahmad, Khalid Mahmood Ashraf, Muhammad Shafiq, Muhammad Ashraf and Muhammad Akmal, International Journal of Modern Physics B, **32** (2018) 1850247

64. First principles study of structural and electronic properties of Ti doped ZnO
T. MUNIR, M. KASHIF, W. HUSSAIN, A. SHAHZAD, M. IMRAN, **A. AHMED**, N. AMIN, N. AHMED, A. HUSSAIN, M. NOREEN, Journal of Ovonic Research, **14** (2018) 333
65. Elastic and mechanical properties of AlZr_3 , AlCu_3 and AlCu_2Zr : First principles study
Ahmad Afaq, Abu Bakar, Muhammad Asif and Bashir Tahir, International Journal of Modern Physics B **32** (2018) 1850300
66. DFT study of SmXO_3 (X=Al and Co) for elastic, mechanical and optical properties
A.Afaq, Abu Bakar, Sajid Anwar, Waheed Anwar and Fazal-e-Aleem International Journal of Modern Physics B, **32** (2018) 1850362

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67. First-Principles study for structural, elastic and mechanical properties of CuCoMnZ (Z=Si, Sn, Sb) Heusler alloys
A Afaq , Shanian MB and Abu Bakar, Mater. Res. Express **6** (2019) 026522
68. Computational investigations of XMgGa (X=Li, Na) half Heusler compounds for thermo-elastic and vibrational properties
A Afaq, M. Rizwan, Abu Bakar, Physica B: Condensed Matter, **554** (2019) 102
69. DFT Study of CuCoMnX (X=Si, Sn, Sb) Quaternary Heusler Alloys for Phonon Spectra
A Afaq, Ayesha Asif, Abu Bakar, M. Rizwan, H. Bushra Munir, Shanian MB, and Muhammad Asif, Modern Physics Letters B, **33** (2019) 1950155
70. Study of thermo-elastic and lattice dynamics properties of half-Heusler compounds XMgAl (X = Li, Na) by computational investigations
A Afaq, Abu Bakar, M. Rizwan, M. Aftab Fareed and H. Bushra Munir and Anila Asif Modern Physics Letters B, **33** (2019) 1950093
71. Reststrahlen Band Studies of RuCrX (X=Si, Ge, Sn) Half Heusler Alloys
A Afaq, Hassan Maaz, Abu Bakar, M. Imran Jamil, Journal of Electronic Materials **48**, (2019) 5323

72. Computational Study of Ru_2TiZ ($Z=Si, Ge, Sn$) for structural, Mechanical and Vibrational properties
Aneeza Iftikhar, **A. Afaq**, Iftikhar Ahmad, Abu Bakar, H. Bushra Munir, Najm Ul Aarifeen and Muhammad Asif, Zeitschrift fur Naturforschung A (ZNA), **74**(6) (2019) 454
73. Computational Investigation of MnNiCuSb alloy for Structural, Elasto-mechanical and vibrational properties
Abu Bakar, Maaz Afzal, Muzaffar Bashir, **A. Afaq**, Aneeza Iftikhar, Fahad Aziz, Muhammad Asif, Modern Physics Letters B, **33**(23) (2019) 1950276
74. First Principles Study of Thermodynamic Properties of $CdxZn_{1-x}O$ ($0 \leq x \leq 1$) Ternary Alloys
Najm ul Aarifeen, **Afaq Ahmad**, H. Bushra Munir and Abu Bakar, Zeitschrift fur Naturforschung A (ZNA), **74** (2019) 1115
75. Quantum photodetachment of hydrogen negative ion in a harmonic potential subjected to static electric field
Azmat Iqbal, Kiran Humayun, Sana Maqsood, Saba Jawaid, **Afaq Ahmad**, Amin Ur Rahman, and Bakht Amin Bacha, Chin. Phys. B, **28** (2019) 023201
76. Reply to “Comment on ‘Gain-assisted superluminal propagation and rotatory drag of photon and surface Plasmon polaritons”
Naveed Khan, Bakht Amin Bacha, Azmat Iqbal, Amin Ur Rahman, and **A. Afaq**, Physical Review A, **99** (2019) 057802
77. First Principles study of thermodynamic properties of Cd-substituted Zn Chalcogenides by employing Quasi Harmonic Debye Model
Najm Ul Aarifeen and **A. Afaq**
Material Research Express, **6** (2019) 116303

2020..... (IF=)

78. *Lattice thermal conductivity of $CdxZn_{1-x}X$ ($X=O, S, Se, Te$) from first principles*
Najm ul Aarifeen, **A. Afaq**,
Materials Chemistry and Physics, **251** (2020) 123099

79. *Theoretical Prediction of Thermodynamic Properties of $CdxZn1-xS$ ($0 \leq x \leq 1$) under the Effects of Pressure (0–10 GPa) and Temperature (0–1200 K)*

Najm ul Aarifeen, **A. Afaq**

Acta Physica Polonica A, 137 (2020) 332

80. *Insight into the structural, vibrational and thermodynamic properties of SmX ($X = S, Se, Te$) chalcogenides: First-principles investigations*

Abu Bakar, **A. Afaq**, M. Faizan Khan, Najm ul Aarifeen, M. Imran Jamil, Muhammad Asif,

Physica B: Phys. of Cond. Matt. 576, (2020) 411715

81. *Reststrahlen band studies in cubic perovskite materials $SmXO_3$ ($X = Al, Co$) by computational investigations*

A Afaq, Abu Bakar, Nimra Khan, and Anila Asif

Int. J. Mod. Phys. B 34 (21) (2020) 2050206

82. *Structural, elasto-mechanical and phonon-related properties of $MnCrP$: A DFT Study*

A Afaq, Abu Bakar, Muhammad Shoaib, Rahsid Ahmed, and Anila Asif,

Int. J. Mod. Phys. B 34 (21) (2020) 2050200

83. *Density functional study of $CoFeCrZ$ ($Z = Al, Si, Ga, Ge$) quaternary Heusler alloys for phonon spectra*

Muhammad Ahmed, **A Afaq**, Abu Bakar, and Muhammad Asif

Int. J. Mod. Phys. B 34 (25), (2020) 2050215

2021.....**(IF=11.537)**

84. *Application of DFT for magnetic anisotropy energy calculations of vanadium ferrite VFe_2O_4*

H. Bushra Munir, **A. Afaq**, Abu Bakar, Iqra Asif, Najm ul Aarifeen, Material Today Communications, 26 (2021) 101763. (IF=2.678)

85. *Optoelectronic Properties of CuCoMnZ (Z=Si, Sn, Sb): A DFT Study*

Abu Bakar, **A. Afaq**, Muhammad Ahmed, Aneeqa Bashir, Muhammad Asif, Journal of Electronic Materials, 50 (2021) 4006. (IF=1.938)

86. *A comprehensive study of Titanium-doped Tin oxide rutile for structural and optical properties*

Abu Bakara, **A. Afaq**, Sidra Latif, Aneezah Iftikhar, Muhammad Asif, Physica B, 619 (2021) 413210. (IF=2.436)

87. *Theoretical predictions of structural electronic and optical properties of vanadium ferrite*

H. Bushra Munir, **A. Afaq**, Abu Bakar, Najm ul Aarifeen, Farid Ullah and Rida Fatima Modern Physics Letters B, 35 (2021) 2150387. (IF=1.224)

88. *First-principles study on the electronic and optical properties of Bi₂WO₆*

Haseeb Ahmad, Rauf Ali, **Afaq Ahmad**, Ata Ulhaq, Muhammad Shoaib, RSC Advances, 11 (2021) 32330. (IF=3.361)

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89. First-principles calculations to investigate elasto-mechanical and opto-electronic properties of pyrochlore oxides X₂Zr₂O₇ (X=La, Nd)

Ali Raza, **A. Afaq**, M. Salman Kiani, Maqsood Ahmed, Abu Bakar, Muhammad Asif, Journal of Materials Research and Technology, **18** (2022) 5005 (IF=6.267).

90. Ab-initio study for the elastic stability, mechanical, electronic and optical properties of RuCrX (X=Si, Ge, Sn) half Heusler alloys, Abu Bakar, **A Afaq**, Muhammad Shoaib, A Dahshan and Muhammad Asif, Physica Scripta, **97** (2022) 075801 (IF=3.081).

91. Pressure-Induced Bandgap Engineering and Tuning Optical Responses of Cd_{0.25}Zn_{0.75}S Alloy for Optoelectronic and Photovoltaic Applications

Muhammad Aamir Iqbal, **Afaq Ahmad**, Maria Malik, Jeong Ryeol Choi, and Phuong V. Pham, Materials, 15 (2022) 2617 (IF=3.623).

92. Effect of pressure on structural, elastic and mechanical properties of cubic perovskites XCoO_3 (X= Nd, Pr) from first-principles investigations
 Abu Bakar, Ayash O. Alrashdi, Muhammad M. Fadhali, **A. Afaq**, H. M. Yakout, Muhammad Asif, Journal of Materials Research and Technology, **19** (2022) 4233 (IF=6.267).
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 Ayash O Alrashdi, Anila Asif, Mohammed M. Fadhali, **A. Afaq**, and Abu Bakar, Journal of Materials Research and Technology, **7** (2022) 45353. (IF=6.267).
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95. First-Principles Investigations of Thermoelectric Behavior of RuCrX (X = Si, Ge, Sn), Muhammad Asif, Ayash O Alrashdi, Mohammed M. Fadhali, **A. Afaq**, and Abu Bakar, ACS Omega, **7** (2022) 45353 (IF=4.132)

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96. Structural stability, mechanical, and optoelectronic properties of A_2TlBiI_6 (A= Cs and Rb) for energy harvesting: A first principles investigation, Anwar ul Haqa, Sadia Sagar Iqbal, **Afaq Ahmad**, Tasawer Shahzad Ahmad, Abu Bakar, Shahid M. Ramay, Journal of Physics and Chemistry of Solids, **176** (2023)111225 (IF= 4.383).
97. Synergistically investigating the structural, magnetic, optoelectronic, and thermo-elastic traits of $\text{LaFe}_{1-x}\text{Ni}_x\text{O}_3$ for novel electronic applications,
 Saad Tariq, Ayash O Alrashdi, **Afaq Ahmed**, and A A Mubarak, Physica Scripta, **98** (2023) 025706 (IF=3.081).
98. Elucidating the Effect of Pressure on Structural, Electronic, Magnetic, Mechanical and Thermal Properties of Mn_2ZrZ (Z=Ge and Si): DFT Overview
 Shamsa Kanwa,1 M. Imran Jamil, Saad Tariq, **Afaq Ahmed**, and Ayash O Alrashdi, ECS Journal of Solid State Science and Technology, **12** (2023) 013003.

99. Precursor concentration-dependent structural, optical and electrical properties of titanium dioxide nanostructures
Asif Majeed, Muhammad Naheem Ahmed , Syed Raza Ali Raza, Abdul Jalil, Ayaz Arif Khan, **Afaq Ahmed**, Materials Chemistry and Physics, **304** (2023) 127786.
100. Opto-electronic and thermoelectric properties of XMgY (X=Li, Na; Y=Al, Ga) alloys: GGA and SCAN based approaches
Abu Bakar, Ayash O. Alrashdi, Saif Ali, Sajid Ur Rehman, **A. Afaq**, Muhammad Asif, Materials Today Communications, **36** (2023) 106451.
101. Optical properties of strontium titanate (STO) thin films using transfer matrix method
M. Asif, **A. Afaq**, M. Amin, Khalid Raouf, Asif Majeed, Muhammad Asif d, Materials Today Communications, **37** (2023) 106966.
102. Cs₂TiRhX₆ (X = Cl, Br, I): promising halide double perovskites for energy harvesting in photovoltaic and thermoelectric applications
Muhammad Amin, Anwar ul Haq, G M Mustifa, **A Afaq**, Shahid M Ramay, Abu baker Ahmed Siddig, Ramesh Sharma and Athar Hanif, Phys. Scr., **98** (2023) 125983.
103. Effects of nonlocal correlation functionals on electron-phonon interactions in NbC
Abu Bakar¹, Muhammad Shahbaz and **A. Afaq**, Phys. Scr., **98** (2023) 105961.
104. Wall Induced-oscillations in Photo detachment of Homo Nuclear Diatomic Molecular Negative ion
105. Saif Rasool, **Afaq Ahmad** and Mohammad Ashraf, PJEST, **4(3)** (2023) 1.
Electron affinity measurement of hydrogen negative ion
Muhammad Usman Ghani, M. Imran Jamil, **Afaq Ahmad**, Saad Tariq, PJEST, **4(2)** (2023) 1.

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106. Transmittance properties of one-dimensional photonic hypercrystals
Ariba Salah, **A. Afaq**, Munazza Zulfiqar Ali, Muhammad Asif, Materials Letters, **364** (2024) 136336.

107. Electronic, phonon and thermoelectric properties of MnCrX (X = As, P, Sb) half Heusler alloys: a DFT study
A Afaq, S E A Akhtar, A Bakar and S M Ramay,
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108. A DFT study to explore structural, elastic, mechanical, phonon, electronic and optical properties of halide perovskites AgXF₃ (X=Be, Ca) with PBEsol, TB-mBJ and SCAN functionals
H. Bushra Munir, A. Afaq, Abdelaziz Gassoumi, Muhammad Ahmed, Abu Bakar,
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109. Determination of the optical properties of tungsten trioxide thin film using the transfer matrix method
M Adnan, M I Jamil, B Ramzan, T Hussain, **A Ahmad** and M U Ghani,
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110. Probing the Structural, Mechanical, Electronic and Optical Properties of TlGeX₃ (X = Cl, Br, I) for Optoelectronic Applications
A Afaq, Abu Bakar, Muhammad Ahmed, Saff e Awal Akhtar, Shahid M. Ramay, Journal of Inorganic and Organometallic Polymers and Materials, **35**(3) (2024)1521.
111. Revealing the remarkably improved structural, phonon, elastic, optoelectronic and thermoelectric properties of TlXF₃(X = Ca, Cd) for energy applications using first-principles approach with hybrid and range-separated hybrid functionals
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112. Superconductivity in LaO: a density functional theory study with local, semilocal, and nonlocal exchange-correlation functionals
Habeb-ur- Rehman, Muhammad S
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113. Theoretical Prediction of the Physical Properties of Novel Fluoro-Perovskites InXF_3 ($X = \text{Sn, Pb}$) for Advanced Optoelectronic and Thermoelectric Applications Using DFT Calculations

Soukaina Bouhmaid, Muhammad Ahmed, Abdelouahid Azouaoui, **A. Afaq**, Larbi Setti, Journal of Inorganic and Organometallic Polymers and Materials, **35** (2025) 6581.

114. Structural, electronic, phonon, thermodynamic and hydrogen storage properties of BeXH_3 ($X = \text{Si, Ge}$) Hydride Perovskites: A DFT approach

A. Afaq, Mehboob Alam, H. Bushra Munir, Abu Bakar, H. Elhosiny Ali, International Journal of Hydrogen Energy, **127** (2025) 127.

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Abu Bakara, Muhammad Shahbaz, **A. Afaq** Journal of Materialia, MTLA **39** (2025) 102329, (IF=2.9)

116. First-Principles insights to probe structural and opto-electronic properties of AgYF_3 ($Y=\text{Mg, Sr}$) halide perovskites with variety of DFT methods

Rida Fatima, **A. Afaq**, Muhammad Ahmed, Abdul Quader, Abu Bakar, Abdulmohsen Alruwaili. Journal of Chemical Physics, **588** (2025) 112443, (IF=3.1)

117. ab-initio insights of BeXH_3 ($X = \text{In, Sn, Sb}$) hydrides for structural, phonon, electronic, thermodynamic and hydrogen storage properties

Abu Bakar, Hafiz Muhammad, **A. Afaq**, Gulnaz K. Toleubay, Erik O. Shalenov, H. Elhosiny Ali, Journal of Energy Storage **132** (2025) 117817, (IF=9.8)

118. A study of quasi-electrostatic and magneto-quasi static wave propagation in a waveguide filled with anisotropic dispersive metamaterial

Yasir Masheh, A. Afaq, Burhan Zamir, Solid State Communications, **404** (2025) 116122.

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119. First principles investigations on physical properties and phonon-mediated superconductivity in CsTaC

Hafiz Muhammad, Abu Bakar, **A. Afaq**, Erik O. Shalenov, H. Elhosiny Ali

Journal of Radiation Physics and Chemistry, Volume **238**, January 2026, 113178,(IF=)

<https://doi.org/10.1016/j.radphyschem.2025.113178>

BOOK PUBLISHED (2024)

Afaq Ahmad, “Interferences in the Photo-detachment of Negative Ion Systems: Two-center Model and Theoretical Imaging Method” Verlag (2010).

CONFERENCE PRESENTATIONS [46]:

1. **Photo-detachment of H^- near a partial reflecting surface using closed orbit**

theory at Seminar Room Block-A, CIIT Lahore on May 05, 2008.

2. **Photo-detachment of H^- near a partial reflecting surface** at Seminar Room Block-A, CIIT Lahore on August 04, 2008.
3. **Interferences in the photo-detachment of Hydrogen Negative ion near an inelastic surface using closed-orbit theory**, 4thInternational Symposium on Quantum Optics, 3-4 August 2009 held at COMSATS Institute of Information Technology Islamabad.
4. **“Classification of partially reflecting surfaces using Photo-detached electron spectrum”**, at Centre of Excellence in Solid State Physics, University of the Punjab Lahore on 29th December 2010.
5. **“A mathematical model to investigate the photo-detachment of a non-linear triatomic negative anion”** at NUST Conference on Applications and Methods of Physics 2011, November 21-22, 2011 held at National University of Science and Technology (NUST) under Centre for Advanced Mathematics and Physics (CAMP) Sector H-12, Islamabad, Pakistan.
6. **Closed Orbit Theory for Hydrogen Fluoride Anion**
Muhammad Hanif, **A. Afaq**, poster presentation at International Scientific Spring – 2012, March 05th - 09th, 2012 held at National Centre for Physics Shahdrah Valley Road, Islamabad.
7. **“Kohn-Sham Equations and their numerical solutions”** at 2ndInternational Workshop on Materials Modeling and Simulations, May 21-24, 2012, held at Department of Physics, University of Malakand.
8. **Structural and Electronic Properties of Ni-Doped ZnO in Zinc-blende Phase: A DFT Investigations**

BukhtiarUlHaq, R. Ahmed, **A. Afaq**, Shaari. A, and M. Zarshenas

The 2nd International Conference on Fundamental and Applied Sciences (ICFAS 2012) Kuala Lumpur, 12-14 June 2012.

9. **Photo-detachment microscopy of the hydrogen negative ion near a dielectric thin film**

Afaq Ahmad

International Conference on Condensed Matter Physics and Engineering, 27-29 Dec. 2012, held at Department of Physics, BahauddinZakria University Multan.

10. **Photo-detachment of a hetero-nuclear diatomic molecular negative ion near an interface**

Afaq Ahmad

3rd International Workshop on Materials Modeling and Simulations (IWMMS-2013), July 3-6, 2013 held at Department of Physics, University of MalakandChakdara, Dir, KPK.

11. **Theoretical study of Photo-detachment Microscopy of H^- ion near an interface**

Maryam Nawaz, **Afaq Ahmad**

International Conference on Solid State Physics (ICSSP13), December 1-6, 2013, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

12. **Band-gap Tailoring of ZnO with the addition of 3d Transition Metal Ions**

Afaq Ahmad, Muhammad Ashraf

International Conference on Solid State Physics (ICSSP13), December 1-6, 2013, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

13. **Structural, elastic and mechanical properties of $XCoO_3$ ($X=Nd, Pr$) from first principle calculations**

Abu Bakar, **A. Afaq**, A Iftikhar, Najm-ulAarifeen

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

14. Spherical Surface Effects in Closed Orbit Theory

A Afaq

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

15. Elastic and mechanical properties of Fe-based Heusler alloys Ru_2FeZ ($Z = Ge, Si, Sn$) using DFT

A Iftikhar, **A. Afaq**, Iftikhar Ahmad, Najm-ul-Arifeen

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore

16. First Principles study of $BiXO_3$ ($X=Fe, Mn, Cr$) for Structural and Magnetic properties

Bushra Munir, **Afaq Ahmad**

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

17. Photodetachment of H^- near a Metal surface: Below Threshold Study

Maryam Ajmal, **A. Afaq**

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

18. Structural, electronic and magnetic properties of $BaUO_3$ by mBJ functional

Najm-ul-Aarifeen, **A. Afaq**, A Iftikhar

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

19. Hydrostatic investigations of structural and opto-electronic properties of $PbZrO_3$: DFT Overview

Saad Tariq, **Afaq Ahmed**

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

20. **SEMICLASSICAL DESCRIPTION OF ION IN A GRADIENT ELECTRIC FIELD**

Ariba Salah, **A. Afaq**

International Conference on Solid State Physics (ICSSP15), December 13-17, 2015, held at Center of Excellence in Solid State Physics, University of the Punjab Lahore.

21. **Modified Closed Orbit Theory to investigate Curvature Effects**

Afaq Ahmad

8th International Meeting on Particles and Fields, on April 20-22, 2016, held at Department of Physics, COMSATS Lahore.

22. **DFT Study on BaUO₃**

Afaq Ahmad

International Conference on Computational Physics, April 09, 2017, held at Department of Physics, University of Lahore.

23. **Photo-detachment of H^- near a spherical solid surface with geometry-dependent classical action**

A Afaq

1st International Conference simulation of Emerging Materials, July 2-4, 2018, held at Department of Physics, Abbottabad University of Science and Technology.

24. **Reststrahlen Band Investigations of Half Heusler Compounds RuCrX (X = Si, Ge, Sn) for FIR-Devices**

Abu Bakar, **A. Afaq**

1st International Conference simulation of Emerging Materials, July 2-4, 2018, held at Department of Physics, Abbottabad University of Science and Technology.

25. DFT and its Application on CuCoMnA (A=Si, Sn, Sb) for FIR-Devices

A Afaq

1st International Physics Conference on Innovation in Materials Science and Nanotechnology, December 18-19, 2018, held at Department of Physics, Lahore Garrison University Lahore.

26. Reststrahlen Band in RuCrX (X=Si, Ge, Sn) Alloys: A DFT Study

Symposium on Semiconductor Physics, November 27, 2019, Virtual University Lahore

27. Reststrahlen Band Investigations in Heusler Alloys for FIR-devices

ICSSP 19, December 9-13, 2019, CSSP Lahore

28. Nanomaterial: A Theoretical Approach

International Workshop on Progress in Nanomaterials and Technology, January 20-22, 2020

29. Density Functional Theory and Its Application to SmXO₃ (X=Al, Co) Pervskites for IR-devices

4th International Conference on Materials Science & Nanotechnology 2020, March 3-5, 2020

30. Electron Affinity for Hydrogen Negative Ion in Photodetachment Microscopy

Emerging Scientists 2020, March 20, 2020, Faisalabad.

31. Photo detachment of H⁻ near two perpendicular elastic interfaces

1st International Congress on Natural Sciences (ICNAS-2021) (Online), 10-12 Sept. 2021, Ata Turk University Turkey.

32. DFT and its application to Lattice Dynamics

33. 2nd International Conference on Advances in Material Science, held online on October 5-6, 2021, Department of Physics, University of Education Lahore.

34. Transfer matrix method and optical properties of a thin-film

International Conference on Innovation in Chemistry and Physics (ICP), March 14-15, 2022 held at University of Education Faisalabad Campus.

35. **First Principles study of optoelectronic and mechanical properties of $\text{Cs}_2\text{AgAlX}_6$ (X= Cl, Br, I) for energy harvesting**
International School on Physics and Applied Discipline (ISPAD), March 14-18, 2022 held at National Centre of Physics (NCP)
36. **Special Functions and their applications**
Capacity Teaching Building Workshop for University Teachers and Graduate Students in Physics, June 23-25, 2022 held at Institute of Physics Gomal University
D. I. Khan.
37. **Transfer matrix method and optical properties of a thin-film**
National One Day Workshop, September 31, 2022 held at Lahore University of Management Sciences (LUMS)
38. **Optical Properties of Perovskite SrTiO_3 Thin Films using Transfer Matrix Method: A Comparative Study**
4th International Workshop on Materials Modeling and Simulation (ICWMMS), October 24-26, 2022 held at University of Malakand, KP.
39. **Optical Band Gap of a Thin Film Using Transfer Matrix Method**
3rd International conference on Advances in Material Sciences (AIMS), December 15-16, 2022 held at University of Education Lahore.
40. **Transfer Matrix Method for Thin Film Optics**
1st National Conference on Emerging Horizons in Science and Technology (NCEHST), December 26-27, 2022.
41. **Theoretical Study of a Thin-Film Optics**
3rd International Conference on Emerging Science and Technologies (ICEST-2023-GIGCCL) to be held on March 1st and 2nd 2023.
42. **THEORETICAL STUDY OF A THIN-FILM OPTICS**
A lecture given at Department of Physics, UAJ&K on 17 March 2023
43. **Quantum Tunneling in Semiconductor Nanostructures by Matrix Method**
5th Annual International Conference on Advances in Materials Science (AIMS-2024) November 27-28, 2024, Department of Physics Division of Science and Technology University of Education, Lahore.
44. **Resonant Tunneling Through Single and Double-barrier Structures**
2nd international conference on “Emerging Trends in Physics”. The conference is scheduled on 6th to 8th of May 2024, IUB Bahawalpur.

45. **OPTICAL PROPERTIES OF THIN FILMS BY MATRICES**

4th International Conference on Emerging Science and Technologies (ICEST-2023-GIGCCL) to be held on March 1st and 2nd 2024

46. **Transfer Matrix Method and Transmission Spectra of Thin Films**

1st International Conference on Emerging Trends in Physics, March, 7-8, 2024,
Department of Physics, UMT Lahore

47. **Optical Properties of Thin Films: A Theoretical Study**

5th International Conference on Emerging Science and Technology and 8th Science Exhibition

Govt. Islamia graduate college Civil Lines. Department of Physics, Lahore, February,24,2025

48. **A Thin film as fabry-Perot Cavity For Optical Fiber Sensing technology**

UMT 2nd International conference on Emerging Trends in Physics (ICP-2025)
Renewable energy Sources and Climate Change Mitigation

Department of Physics & department of Mathematics, School of science, UMT, Lahore, April 14-15, 2025

M. PHIL THESES SUPERVISED: [109]

The following M.Phil students' theses have been supervised:

Session 2008-2010

1. **Sadia Ashiq** (SSP0802, PU Lahore)

Thesis Title: Bond length calculation of a diatomic anion and its classical limit using two center model.

2. **M. Asif Toseef** (SSP0810, PU Lahore)

Thesis Title: Theoretical investigation of structural and Optical properties of $\text{Sc}_{1-x}\text{Y}_x\text{N}$.

3. **Farooq Khan** (SSP0823, PU Lahore)

Thesis Title: Interferences in photo-detachment of Non-linear triatomic anion.

Session 2009-2011

4. **Bakhtiar Ul Haq** (SSP0915, PU Lahore)

Thesis Title: Characterization of Co doped ZnO based diluted magnetic semiconductors.

5. **Marayam Nawaz** (SSP0903, PU Lahore)

Thesis Title: Photo-detachment of hetero-nuclear diatomic anions near a reflecting wall.

6. **M. Hanif** (SSP0909, PU Lahore)

Thesis Title: Photo-detachment of hetero-nuclear diatomic anions using closed-orbit theory.

7. **M. Fahim Afsar** (SSP0916, PU Lahore)

Thesis Title: Analysis of Floquet Formulation of Time-Dependent Density-Functional Theory.

Session 2010-2012

8. **Ayesha Amjad** (SSP1001, PU Lahore)

Thesis Title: Photo-detachment of Hydrogen Halide Anions near a wall.

9. **Tayyiba Fiazi** (SSP1004, PU Lahore)

Thesis Title: Photo-detachment of H^- near a dielectric thin film.

10. **Sanober Kanwal** (SSP1013, PU Lahore)

Thesis Title: Interferences in photo-detachment of a tri-atomic negative ion near a reflecting wall.

11. **Muhammad Ashraf** (SSP1019, PU Lahore)

Thesis Title: Bandgap Tailoring of ZnO with the Addition of 3d Transition Metal Ions.

Session 2011-2013

12. **Salman Ahmad** (SSP1109, PU Lahore)

Thesis Title: Structural, electronic and magnetic properties of Cr-doped PbS alloys.

13. **Aneela Arshad** (SSP1105, PU Lahore)

Thesis Title: Structural and Optical Properties of BP, BSb, and their alloys.

14. **Farhan Shabir Ahmad** (SSP1106, PU Lahore)

Thesis Title: Structural and Optical Properties of XZrO_3 (X=Ba, Sr, Pb) perovskite crystals.

15. **Qandeel Fida** (SSP1107, PU Lahore)

Thesis Title: Photo-detachment Microscopy of H^- near a Dielectric Slab.

16. **Ali Asad** (SSP1117, PU Lahore)

Thesis Title: Pressure dependent Structural and Optical Properties of XSe (X=Zn, Cd).

Session 2012-2014

17. **Hafsa Naz** (SSP1209, PU Lahore)

Thesis Title: Polarization-dependent photo-detachment of Hydrogen negative ion

18. **Muhammad Saad Tariq Mirza** (SSP1212, PU Lahore)

Thesis Title: Structural and Electronic properties of cubic Pervoskites XZrO_3 (X=Ba, Sr, Pb) under pressure: A DFT Study

19. Ghazanfar Nazir (SSP1213, PU Lahore)

Thesis Title: Optical Properties of cubic Perovskites $XZrO_3$ ($X=Ba, Sr, Pb$) under pressure: A DFT Study

Session 2013-2015

20. Maryam Ajmal (SSP1301, PU Lahore)

Thesis Title: Photodetachment Cross Section of Hydrogen Negative Ion below Threshold Energy

21. Rafia Ifikhar (SSP1302, PU Lahore)

Thesis Title: Semi-classical description of Fullerene C_{60} and Metallic Clusters

22. Anam Lashari (SSP1303, PU Lahore)

Thesis Title: Photodetachment of H^- in a Circular Microcavity

23. Bilal Adeel Kazmi (SSP1305, PU Lahore)

Thesis Title: Structural and Electronic Properties of $Zn_{1-x}Cd_xSe$

24. Ariba Salah (SSP1306, PU Lahore)

Thesis Title: Influence of a Gradient Electric Field on H^- A semi-classical Description

25. Muhammad Saad Tanvir (SSP1311, PU Lahore)

Thesis Title: Photo-detachment of H^- near a Non-absorbing Metal Surface

26. Hafiza Bushra Munir (SSP1315, PU Lahore)

Thesis Title: Structural and Magnetic Properties of $BiXO_3$ ($X = Fe, Cr, Mn$)

27. Abdul Muteen (SSP1323, PU Lahore)

Thesis Title: Photo-detachment of H^- in a soft microcavity.

Session 2014-2016

28. Abu Bakar (SSP1418, PU Lahore)

Thesis Title: First Principles Study of Elastic and Mechanical Properties of $AlZr_3$, $AlCu_3$, and $AlCu_2Zr$

Session 2015-2017

29. Ameer Hamza (SSP 1501, PU Lahore)

Thesis Title: DFT study on Ru_2FeZ ($Z=Si, Ge$) Heusler Alloys for Structural and Thermodynamic Properties

30. Shafaq Naseer (SSP 1503, PU Lahore)

Thesis Title: Structural and Electronic Properties of Zn-substituted CdS Alloys under Pressure

31. Shaista Itefaq (SSP 1507, PU Lahore)

Thesis Title: Photo-detachment of H^- Ion near a Soft Spherical Surface

32. Kiran Sijawal (SSP 1516, PU Lahore)

Thesis Title: Structural and Electronic Properties of Zn-substituted CdTe Alloys under Pressure

33. Muhammad Rizwan khan (SSP 1519, PU Lahore)

Thesis Title: DFT study on Ru_2FeX ($X=Si, Ge$) Heusler Alloys for Elastic and Vibrational Properties

Session 2016-2018

34. Muhammad Aftab Fareed (SSP1601F16, PU Lahore)

Thesis Title: Lattice Dynamics of $XMgAl$ ($X=Li, Na$) Alloys

35. Ayesha Asif (SSP1604F16, PU Lahore)

Thesis Title: Computational Reststrahlen Band investigations in $CuCoMnA$ ($A=Si, Sn, Sb$) FIR-Devices

36. Hafiz Shamsheer Islam (SSP1606F16, PU Lahore)

Thesis Title: Photo Detachment of Hydrogen Anion near a Spherical Surface and Study of Geometry Dependent Classical Action using TIM

37. Shanian (SSP1608F16, PU Lahore)

Thesis Title: Computational Investigation of structural elastic and mechanical properties of $CuCoMnZ$ ($Z=Si, Sn, Sb$) Alloys

38. Sidra Latif (SSP1610F16, PU Lahore)

Thesis Title: Structural and Optical Properties of Rutile $Sn_{1-x}Ti_xO_2$ ($0 < x < 1$):
A DFT Study

39. Iqra Asif (SSP1612F16, PU Lahore)

Thesis Title: Structural, Electronic and Magnetic Properties of VFe_2O_4 : A DFT Study

40. Khush Bakht Waris Ali (SSP1618F16, PU Lahore)

Thesis Title: Energy Loss Function for Metals (Fe, Mo) and Insulators (BaTiO₃, SmAlO₃)

41. Muhammad Sabeeh Ashraf (SSP1603FF16, PU Lahore)

Thesis Title:

42. Aamer Zaman (SSP1621F16, PU Lahore)

Thesis Title: Plane Wave Propagation through Multilayer system

Session 2017-2019

43. Muhammad Ahmed (SSP02F17, PU Lahore)

Thesis Title: Reststrahlen Band Investigations of CoFeCrZ (Z=Al, Si, Ga and Ge) for FIR Applications

44. Rida Fatima (SSP03F17, PU Lahore)

Thesis Title: Temperature Dependent Structural Properties of VFe₂O₄: A DFT Study

45. Tahir Shakeel (SSP09F17, PU Lahore)

Thesis Title: Computational Study of Elastic and Mechanical Properties of RuCrX (X=Si, Ge, Sn)

46. Nimra Khan (SSP19F17, PU Lahore)

Thesis Title: Vibrational Properties of SmXO₃ (X=Al, Co): A DFT Study

47. Farid Ullah (SSP20F17, PU Lahore)

Thesis Title: Magnetic Anisotropy Energy of Vanadium Ferrite (VFe₂O₄): A DFT Study

48. Said Alam (SSP21F17, PU Lahore)

Thesis Title: Complex Conductivity Dependent Birefringence Via Rotatory Photon Drag Through a Chiral Metallic Medium

49. Allah Ditta (SSPR02F17, CSSP, PU, Lahore) (2019)

Thesis Title: DFT Study for Electronic and Optical Properties of Pyrochlore X₂Zr₂O₇ (X=La, Nd)

50. Amir Junaid (SSPR21F17, CSSP, PU, Lahore) (2019)

Thesis Title: Optical Properties of Chromium Substituted Zinc Sulfide (ZnS): A DFT Study

- 51. Muhammad Ashfaq** (SSPR33F17, CSSP, PU, Lahore) (2019)
Thesis Title: Optical Properties of Cr-Substituted ZnSe Using Density Functional Theory
- 52. Zanib Saeed Khan** (SSPR23F17, PU Lahore)
Thesis Title: H Photo-detachment in a Wall-Field System: A QM Study
- 53. Muhammad Waheed Arshad** (SSPR36F17, CSSP, PU, Lahore) (2019)
Thesis Title: Optical Properties of Cd-Substituted ZnSe Using Density Functional Theory
- 54. Muhammad Aleem** (SSPR41F17, CSSP, PU, Lahore) (2019)
Thesis Title: Optical Properties of Cadmium (Cd) Substituted Zinc Sulfide (ZnS): A DFT Study
- 55. Ayesha Sadiqah** (SSPR46F17, PU Lahore)
Thesis Title: H Photo-detachment in a Wall-Field System: A COT Study
- 56. Inaam Rasool** (SSPR48F17, CSSP, PU, Lahore) (2019)
Thesis Title: Structural and Optoelectronic of MnCrP: A DFT Study
- 57. Ali Raza** (SSPR66F17, CSSP, PU, Lahore) (2019)
Thesis Title: DFT Study for Structural, Elastic and Mechanical Properties of $\text{La}_2\text{Zr}_2\text{O}_7$ Pyrochlores
- 58. Muhammad Shoaib** (SSPR67F17, CSSP, PU, Lahore) (2019)
Thesis Title: DFT Study for Elastic, Mechanical and Vibrational Properties of MnCrP
- 59. Sadam Hussain** (SSPR75F17, PU Lahore)
Thesis Title: Reststrahlen Band investigations in Neptunium based Chalcogenides: A DFT Study
- 60. Saddam Hussain** (SSPR99F17, PU Lahore)
Thesis Title: Photon Drag and Polarization Rotation of Slow Light in a Condensed Medium

Session 2018-2020

- 61. Yasir Masheh** (SSP02F18, PU Lahore)
Thesis Title: Propagation characteristics of electromagnetic waves in a rectangular waveguide filled with an anisotropic metamaterial
- 62. Muhammad Asad Ullah** (SSP16F18, PU Lahore)

Thesis Title: Structural, Elastic and Mechanical Properties of $\text{Nd}_2\text{Zr}_2\text{O}_7$ Pyrochlore: A DFT Study

63. Atiq Ur Rehman (SSP19F18, PU Lahore)

Thesis Title: DFT Study of Infrared Optical Properties of Ruc

64. Marwan Alam (SSP21F18, PU Lahore)

Thesis Title: First-Principles Study of Janus Monolayer SnSSe

65. Rizwan Hussain (SSP27F18, PU Lahore)

Thesis Title: Structural, Electronic and Magnetic Properties of ZnFe_2O_4 : A DFT Study

66. Mehran Ullah (SSP24F18, PU Lahore)

Thesis Title: DFT STUDY OPTICAL PROPERTIES OF XC (X = Ag, Pd)

67. Hafiz Muhammad (SSPR79F18, PU Lahore)

Thesis Title: Electron Affinity Measurement of Hydrogen Negative Ion near an Interface

68. Muhammad Hammad (SSPR24F18, PU Lahore)

Thesis Title: Photo-detachment of Hydrogen Negative Ion inside two Parallel Interfaces:
A Numerical Analysis

69. Muhammad Mohsan Aslam (SSPR19F18, PU Lahore)

Thesis Title: Plane wave Reflection at the Interface Between two Isotropic Media

70. Shehzad Basheer (SSPR10F18, PU Lahore)

Thesis Title: Measurement of Brewster Angle for Different Interfaces

Session 2019-2021

71. Ayesha Ashraff (SSP02F19, PU Lahore)

Thesis Title: Interference in the photo-detachment cross section H near two perpendicular walls

72. Chanda Talib (SSP06F19, PU Lahore)

Thesis Title:

73. Zeenat Mushtaq (SSP12F19, PU Lahore)

Thesis Title:

74. Sanan Ahmad, (SSP11F19, PU Lahore)

Thesis Title: Photo-detachment of a Hetro-Nuclear Diatomic Molecular Negative Ion

near a Surface

75. Salah ud Din (SSP23F19, PU Lahore)

Thesis Title: Photo-detachment of diatomic molecular negative ion

76. Muhammad Ali (SSPR27F19, PU Lahore)

Thesis Title:

77. Awais Ali (SSPR167F19, PU Lahore)

Thesis Title:

78. Aithsam Asif (SSPR187F19, PU Lahore)

Thesis Title:

Session 2020-2022

79. Habeeb-ur Rehman (M.Phil-SSP01F20)

Thesis Title: DFT study of superconductivity in LaO: local and non local functionals

80. Muhammad Ashraf (M.Phil-SSP04F20)

Thesis Title: Photodetachment of a homo-nuclear diatomic molecular negative ion near the wall surface

81. Amina Alam (M.Phil-SSP05F20)

Thesis Title: Exploring the Elastic and Mechanical Properties of Oxide Perovskite -LaFeO₃

82. Saff-e-Awal (M.Phil-SSP12F20)

Thesis Title: Effect of XC functionals on electronic, magnetic, and thermoelectric properties of 1T-CrO₂ for application of spintronics

83. Khalid Raouf (M.Phil-SSP017F20)

Thesis Title: Optical Properties of Perovskite SrTiO₃ Thin Films using Transfer Matrix Method

84. Hamza Khalid (MPhil_SSPR128F20)

Thesis Title: Review of Hagen-Rubens Relation Beyond Far Infrared Region

85. Husnain Ahmed Zia (MPhil_SSPR52F20)

Thesis Title: Optical Band Dap in SrTiO₃ Crystalline Think Films: A

Comparative Study

86. Umair Mumtaz (MPhil_SSPR76RF20)

Thesis Title: Structural and Optical Properties of $LaFe_{1-x}Cr_xO_3$ (x=0-100%): A DFT Study

87. Usama Azhar (MPhil_SSPR140F20)

Thesis Title: Structural and Electronic Properties of Cubic Perovskite BaThO₃ Under Pressure: A DFT study

88. Usama Subak Majid (M. Phil_SSPR90F20)

Thesis Title: Structural and Electronic Properties of SrTiO₃: A Computational Study

Session 2021-2023

89. Muhammad Shan (SSP03F21):

Thesis Title: Study of Skin Effect in Metals with Generalized Ohm's Law

90. Muhammad Nasir (SSP04F21):

Thesis Title: Electromagnetic Wave Propagation in Hollow and Filled rectangular Waveguides

91. Usman Ali Shah (SSP18F21):

Thesis Title: Optical Band Gaps of Zinc Telluride (ZnTe) Thin Films: A Theoretical Study

92. Muhammad Ahmad (SSP16F21):

Thesis Title: A Photonic Hyper-crystal: A New Artificial Optical Medium

93. Yasmeen Ahmad (SSP02F21):

Thesis Title: Reflection and Transmission at a moving interface

94. Noreen Ayesha (SSP09F21):

Thesis Title: Wave Propagation in a Hyperbolic Metamaterial

95. Jahanzaib (SSPR181F21)

Thesis Title: A DFT study of elastic and mechanical properties of Half-Heusler Alloys RuVX (X=P, Sb, As)

96. Muhammad Usman (SSPR128F21)

Thesis Title: Extended irreversible thermodynamics and skin effect

97. M. Awais (SSPR99F21)

Thesis Title: DFT study of Phonon properties of Half-Heusler Alloys MnCrX=
(X=P, Sb, As)

98. Muhammad Abrar Hussain Saqib (SSPR40F21)

Thesis Title: A DFT study of elastic and mechanical properties of Half-Heusler Alloys MnCrX (X=P, Sb, As)

Session 2022-2024

99. Shahzad Maqbool (SSP16F22):

Thesis Title: Resonant Tunneling Through Single and Double-Barrier Structures

100. Muhammad Shahzad, (SSPR181F22)

Thesis Title : Investigation of Elasto-Mechanical Properties of LuNiSb using DFT

101. Shahdat Ali, (SSPR1201F22)

Thesis Title: Synthesis and Characterization of Zinc Cobalt Sulfide-Graphitic Carbon Nitride (ZCS-GCN) Nanostructures for Enhanced Energy Storage Applications

102. Mahboob Alam, (SSPR128F22)

Thesis Title: Investigation of Elasto-Mechanical Properties of TmNiSb using DFT

103. Muhammad Irfan, (SSPR82F22)

Thesis Title: Transmission Through Layered Media

Session 2023-2025

104. M. Usman (SSP18F23)

Thesis Title: Investigating Tunneling time in Quantum systems with Step Potential Barriers

105. M. Zia Ur Rehman (SSP14F23)

Thesis Title: Electron Transmission Probability in a One-Dimensional Crystal with Triangular Potential Barriers

106. Maryam Yousaf (SSP15F23)

Thesis Title: Optical Properties of Tungsten Trioxide WO₃ Thin films Experimental and Theoretical Study

107. Umaima Shahid (SSPR87F23)

Thesis Title: Optical Characterization of a ZnTe film using Transfer Matric Method

108. Tayyab Ahmad (SSPR82F22)

Thesis Title: Electron transmission Probability in a One-Demensional Crystal with Sinusoidal potential Barriers

109. Arslan Afzal (SSPR16F23)

Thesis Title: Tunneling Time by Steinberg and Ramsey Approaches

Co-supervised the following M. Phil student's theses: [16]

110. M Musharaf Ansari (CHEP, PU, Lahore) (2009)

Thesis Title: Photo-detachment of **H** near an elastic wall using theoretical imaging method

111. Azmat Iqbal (CHEP, PU, Lahore) (2009)

Thesis Title: Photo-detachment of **H** near an elastic wall using closed orbit theory

112. Waheed Anwar (PHP01153145, UOL, Lahore) (2017)

Thesis Title: Structural and Optical Properties of SmXO_3 ($X=\text{Al, Co}$) Cubic Pervoskites: A First Principles Study

113. Sajid Anwar (PHP01153150, UOL, Lahore) (2017)

Thesis Title: Structural, Elastic and Mechanical Properties of SmXO_3 ($X=\text{Al, Co}$) Cubic Pervoskites: A First Principles Study

114. Shumaila Nazir (F2016139008, UMT, Lahore) (2018)

Thesis Title: Structural, Electronic and Optical Properties of BaZrO_3 and SrZrO_3 : A DFT Study

115. Hassan Maaz (F2016139002, UMT, Lahore) (2018)

Thesis Title: Reststrahlen Band Investigation of Half-Heusler Compounds RuCrZ ($Z = \text{Si, Ge and Sn}$) for Far-Infrared Devices

116. Muhammad Faizan Khan (F2016139010, UMT, Lahore) (2018)

Thesis Title: Vibrational and Thermodynamical Properties of SmX ($X = \text{S, Se, and Te}$) Chalcogenides: A DFT Study

117. Maaz Afzal (PU, Lahore) (2019)

Thesis Title: Computationally Calculated Structural, Elastic and Vibrational Properties for Experimentally Observed Quaternary Heusler Alloy MnNiCuSb

Ph. D. STUDENTS [5+12]:

Supervised [12]

1. **Ghulam Murtaza** (03-01-2012) (Department of Physics, Hazara University, Pakistan)
Thesis Title: First Principles Study of Optoelectronic Properties of Cubic Perovskites
2. **Amin-ur-Rehman** (13-06-2012) (Department of Physics, Hazara University Pakistan)
Thesis Title: Photo-detachment of Linear Negative Ions Systems
3. **Muhammad Hanif** (Department of Physics, Hazara University, Pakistan) (2015)
Thesis Title: Photo-detachment of negative ions near spherical surfaces
4. **Bukhtiar Ul Haq** (Department of Physics, University Technology Malaysia (UTM) (2015)

Thesis Title: Study of doping effect of transition metals (Ni, Mn, Co, Fe, V, and Cr etc.) in ZnO.

5. **Aneza Iftikhar** (PHD1303) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: DFT CALCULATIONS of Ru AND Rh BASED HEUSLER ALLOYS
6. **Najam Ul Arfeen** (PHD1403) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: Theoretical investigations of thermodynamic properties of Cd substituted Zn-Chalcogenides
7. **Hafiza Bushra Munir** (PhD1605) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: First principles investigations on structural and magnetic properties of spinel ferrites (XFe_2O_4 : X = V; Mo; Zn)
8. **Abu Bakar** (PhD1704) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: Theoretical Investigations of Electron-Phonon Interactions in Metal Carbides
9. **Muhammad Saad Tariq Mirza (PhD1708)** (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: tuning the Physical Attributes of Lanthanum Based Perovskites by Substituting d-Orbital elements Using Density functional theory
10. **Shamsa Kanwal** (Department of Physics, School of Science University of Management and Technology Lahore)
Thesis Title: Pressure-dependent Structural and Magnetic Properties of Mn-based Heusler Alloys: A DFT Study

11. **Asim Nisan Sheikh** (Department of Physics, School of Science University of Management and Technology Lahore)
Thesis Title: Computational Study on Ru and Rh based Heusler Alloys for their Structural, electrical and Electrical Responses

12. **Ariba Salah** (PhD1504) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: Analysis of transmission Properties of Photonic Hypercrystals
Transmission Properties of Photonic Hyper-crystals

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Supervising [05]

1. **Ayesha Aftab** (PhD1802) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: -----

2. **M. Ashraf** (PhD-SSP03F21) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: -----

3. **Yasir Masih** (PhD-SSP02F21) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: Theoretical Analysis of Wave Propagation in Filled Waveguide Structures for Microwave Applications

4. **M. Waseem** (PhD-SSP04F23) (Center of Excellence in Solid State Physics, University of the Punjab Lahore Pakistan)
Thesis Title: -----

5. **Husnain Ahmed Zia** (PhD-SSP16-F22) (Center of Excellence in Solid State Physics,
University of the Punjab Lahore Pakistan)

Thesis Title: Theoretical Study of Optical Multilayer Thin Films and
One-Dimensional Quantum Systems.

REFERENCES:

1. **Prof. Dr. Khaleeq-Ur-Rehman**, Rector, Green International University Lahore.
(Cell No. 0300-4445266)
2. **Prof. Dr. Iftikhar Ahmad**, VC Gomal University, DI Khan, KPK, Pakistan.
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