Curriculum vitae

SALEEM AYAZ KHAN

Date Of Birth: April 12th 1982
Nationality: Pakistan
Permanent residency: Czech Republic
Email: khan@ntc.zcu.cz

OFFICIAL ADDRESS

New Technologies - Research Center,
University of West Bohemia,
Univerzitni 8, 306 14 Pilsen,
Czech Republic, (+420) 377634793

HOME ADDRESS

Borska 2756/53
city code: 30 100 Pilsen,
Czech Republic,
(+420) 777083956

Research area

Ab initio calculations of electronic structure, optical, magnetic and thermoelectric properties of technologically interesting materials.

Current Status

Working as researcher in Project Computational and experimental design of advanced materials with new functionalities CEDAMNF, Reg. No. CZ.02.1.01/0.0/0.0/15_003/0000358, co-funded by the European Regional Development Fund.

Current research projects

- Effect of correlations on magnetocrystalline anisotropy of FePt
- Magnetic properties of $Fe_{0.5}Pt_{0.5}$ substitutional alloys: local environment effect.
- Disorder broadening of core levels in FePt: comparison between different levels
- Study of Fe embedded surface layer of Pt(111) in order to explain the experimental data.
- Ab initio x-ray absorption spectroscopy of B doped Si(111) in order to study interesting experimental data.
- DMFT treatment for reliable MCA energy of FeO, CoO, NiO and FePt.
- Luminescence of $\beta - SiAlON : Eu^{2+}$ phosphors: DFT study

EDUCATION

2018	PostDoc	University of West Bohemia. Czech Republic
2017	PhD.	University of West Bohemia. Czech Republic
2011	M.Phill.	Hazara University, Pakistan
2008	M.Sc.	University of Malakand, Pakistan
2003	B.Sc.	University of Peshawar, Pakistan
2000	F.Sc.	BISE Peshawar, Pakistan
1998	SSc.	BISE Peshawar, Pakistan

Master in Philosophy thesis title (M. Phil):

Critical radii of cubic perovskites: A theoretical study.

Doctor in Philosophy thesis title (Ph.D):

Electronic structure calculations as an aid to study structure and magnetism of layered materials.

EXPERIENCE

Teaching; Teaching experience in different graduate and undergraduate institutes during 2007-2011.

Proficiencies:

- **Wien2k Code**
- **BoltzTraP Code**
- **Elastic Code**
- **ELK Code**
- **SPRKKR Code**
- **VASP Code**
- **Exciting Code**

Subjects studied:

Quantum mechanics, statistical mechanics, Quantum optics Magnetism, Electronics
mathematical method Plasma physics, Modern physics Nuclear physics
of physics, Optical properties, Electro dynamics, Electro magnetic theory
Classical mechanics, Solid state physics

Research stays and collaborations:

- Autum School on dynamical mean field approach with predictive power for strongly correlated Electrons FZ, Jülich, Germany, 2014.
- Short term scientific visit (15 days) to Institute of Materials Chemistry, TU Vienna, Austria "Collaboration with Prof. Peter Blaha on advance properties of WIEN2K for FePt bulk and nanostructures", 2015.

- Hands-on course Introduction to the application of ab-initio methods in spectroscopy, New Technologies Research Centre, University of West Bohemia Czech Republic, 2015.
- Short term scientific visit (10 days) to the group Prof. Peter Blaha in Institute of Materials Chemistry, TU Vienna, Austria, "Collaboration with Prof. Peter Blaha on Fe/Pt(111) low dimensional nanostructures", 2016.
- Winter school on the fundamentals and applications of ab-initio methods in spectroscopy, Applied Physics Faculty of the University of Nova Gorica, Ajdovščina, Slovenia, 2016.
- Winter School "Computational Magnetism" at the Vienna University of Technology, Austria, 2017.
- Success-2017, Les Houches, France.
- Workshop on high correlating system, Dresden (Germany), 2017.
- Short term scientific visit (7 days) to Uppsala university Sweden "Collaboration with Prof. Igor Di Marco and Johan Schött on DMFT to calculate magnetic anisotropy of FePt", 2017.
- Training school on spectroscopy codes organized by European Cooperation of Science and Technology, Sofia (Bulgaria), 2018.
- Workshop and hands-on school on the FP-LMTO method and DMFT, Santo Stefano di Sessanio (Italy) 2018.

Conferences/Workshops Attended:

- DPG-Frühjahrstagung (DPG Spring Meeting) Dresden, Germany, 2014.
- S. A. Khan, O. Šipr "*Theoretical investigation of electronic structure and spectroscopic properties of CdO nanosheet*" Autum School on correlated Electrons, FZ, Jülich, Germany, 2014, (poster presentation).
- S. A. Khan, J. Minár, O. Šipr "*Magnetism of Fe/Pt surface alloys and Fe/Pt nanostructures embedded in Pt(111) via ab initio calculations*" Hands-on course Introduction to the application of ab-initio methods in spectroscopy, New Technologies Research Centre, University of West Bohemia Czech Republic, 2015, (poster presentation).
- S. A. Khan, J. Minár, O. Šipr "*Magnetism of Fe/Pt surface alloys and Fe/Pt nanostructures embedded in Pt(111) via ab initio calculations*" DPG conference in Berlin, Germany, 2015, (Oral talk).
- S. A. Khan, P. Blaha, H. Ebert, J. Minár, O. Šipr "*Magnetocrystalline anisotropy of FePt: a detailed view.*" Psi-k 2015 conference, San Sebastian, Spain, 2015, (poster presentation).
- S. A. Khan, P. Blaha, H. Ebert, J. Minár, O. Šipr "*Magnetocrystalline anisotropy of FePt: a detailed view.*" Winter school on the fundamentals and applications of ab-initio methods in spectroscopy, Applied Physics Faculty of the University of Nova Gorica, Ajdovščina, Slovenia, 2016, (poster presentation).

- S. A. Khan, P. Blaha, H. Ebert, J. Minár, O. Šipr "*A detailed view on the effect of the spin-orbit coupling on the magnetocrystalline anisotropy: case study of FePt*" DPG conference in Regensburg, 2016, (Oral talk).
- S. A. Khan, J. Minár, H. Ebert, P. Blaha, O. Šipr "*Local environment effects in the magnetic properties and electronic structure of disordered FePt*" ViCoM Winter School on Magnetism, 2017, (Oral talk).
- S. A. Khan, J. Minár, H. Ebert, P. Blaha, O. Šipr "*Local environment effects in the magnetic properties and electronic structure of disordered FePt*" DPG conference in Dresden, Germany, 2017, (Oral talk).
- S. A. Khan, M. Vondráček, P. Blaha, K. Horáková, O. Šipr, V. Cháb "*Local geometry around B atoms in B/Si(111) from polarized x-ray absorption spectroscopy*" Success-2017, Les Houches, France, (poster presentation).
- S. A. Khan, J. Minár, H. Ebert, P. Blaha, O. Šipr "*Disorder broadening of core levels in FePt: comparison between different levels* Workshop on high correlating system, Dresden, Germany, 2017, (poster presentation).
- S. A. Khan, J. Xu, J. Schött, I. Di Marco, O. Šipr, J. Minár, "*Magnetocrystalline anisotropy of FePt: LDA+DMFT study*" DPG conference in Berlin, Germany, 2018, (Oral talk).
- S. A. Khan, J. Xu, J. Schött, I. Di Marco, O. Šipr, J. Minár, "*Magnetocrystalline anisotropy of FePt: LDA+DMFT study*" International Symposium on Condensed Matter Physics and Nano Technology in The Women University Multan, Pakistan, 2018 (Oral talk as invited speaker).
- S. A. Khan, J. Xu, J. Schött, I. Di Marco, O. Šipr, J. Minár, "*Magnetocrystalline anisotropy of FePt: LDA+DMFT study*" Workshop and hands-on school on the FP-LMTO method and DMFT, Santo Stefano di Sessanio, Italy, 2018, (Oral talk).
- S. A. Khan, J. Xu, J. Schött, I. Di Marco, O. Šipr, J. Minár, "*Effect of correlations on magnetocrystalline anisotropy of FePt*" Autum School on correlated Electrons, FZ, Jülich, Germany, 2018, (poster presentation).
- S. A. Khan, J. Xu, J. Schött, I. Di Marco, O. Šipr, J. Minár, "*Effect of correlations on magnetocrystalline anisotropy of FePt*" NTC Annual Offsite Meeting 2018 Nečtiny, Czech Republic (poster presentation).
- S. A. Khan, O. Šipr, R. Niklaus, W. Schnick, J. Minár, "*Luminescence of* $\beta - SiAlON : Eu^{2+}$ *phosphors: DFT study*" DPG conference in Regensburg, 2019.
- S. A. Khan, O. Caha, O. Rader, G. Springholz, J. Minár, "*Magnetocrystalline Anisotropy of Mn Induced* Bi_2X_3 *(X=Se, Te) Heterostructure: DFT Study*" Magnetics and Optics Research International Symposium 2019, Charles University, Prague, Czech Republic (poster presentation).

LIST OF PUBLICATIONS

Publications: 65
Citations (Without self) 350
h-index 12
website: https://www.researchgate.net/profile/Saleem_Khan11

Selected publications

1. S. A. Khan, P. Blaha, H. Ebert, J. Minár, O. Šipr: *Magnetocrystalline anisotropy of FePt: a detailed view.* Phys. Rev. B. 94 (2016) 144436.
2. S. A. Khan, P. Blaha, H. Ebert, J. Minár, O. Šipr: *Local environment effects in magnetic properties and electronic structure of disordered FePt.* Phys. Rev. B. 95 (2017) 014408.
3. E. D. L. Rienks, S. Wimmer, P. S. Mandal, O. Caha, J. Ruzicka, A. Ney, H. Steiner, V. V. Volobuev, H. Groiss, M. Albu, S. A. Khan, J. Minár, H. Ebert, G. Bauer, A. Varykhalov, J. Sánchez-Barriga, O. Rader, G. Springholz :*Large magnetic gap at the Dirac point in a Mn-induced Bi_2Te_3 heterostructure* Nature 576 (2019) 423.
4. S. A. Khan, M. Vondráček, P. Blaha, K. Horáková, J. Minár, O. Šipr, V. Cháb :*Local geometry around B atoms in B/Si(111) from polarized x-ray absorption spectroscopy* J. Phys.: Condens. Matter 32 (2020) 045901.

Publications 2013-2018

1. S. A. Khan, A. H. Reshak: *First Principle Study of Electronic Structure, Chemical Bonding and Optical Properties of 5-azido-1H-tetrazole.* Int. J. Electrochem. Sci., 8 (2013) 9459.
2. A. H. Reshak, S. A. Khan: *Density of electronic states and dispersion of optical functions of defect chalcopyrite $CdGa_2X_4(X = S, Se)$: DFT study.* Mater. Res. Bull. 48 (2013) 4555.
3. A. H. Reshak, S. A. Khan: *Electronic structure and optical properties of $In_2X_2O_7(X = Si, Ge, Sn)$ from direct to indirect gap: An ab initio study.* Comput. Mater. Sci. 78 (2013) 91.
4. A. H. Reshak, S. A. Khan: *NaAuS chicken-wire-like semiconductor: Electronic structure and optical properties.* J. Alloys Compd. 582 (2014) 6.
5. A. H. Reshak, S. A. Khan: *Thermoelectric properties, electronic structure and optoelectronic properties of anisotropic $Ba_2Tl_2CuO_6$ single crystal from DFT approach.* J. Magn. Magn. Mater. 354 (2014) 216.
6. A. H. Reshak, S. A. Khan: *Dispersion of the second harmonic generation from $CdGa_2X_4(X = S, Se)$ defect chalcopyrite: DFT calculations.* J. Alloys. Compd. 595 (2014) 125.
7. A. H. Reshak, S. A. Khan: *Electronic band structure and specific features of AA- and AB-stacking of carbon nitride (C3N4): DFT calculation.* RSC Advances, 4 (2014) 6957.
8. S. A. Khan, A. H. Reshak, Z. A. Alahmed:*Electronic band structure and optoelectronic properties of $SrCu_2X_2(X = As, Sb)$: DFT calculation.* J. Mater. Sci. 49 (2014) 5208.
9. S. A. Khan, A.H. Reshak: *Optoelectronic and transport properties of Zintl phase $KBa_2Cd_2Sb_3$*

compound. Comput. Mater. Sci. 95 (2014) 328.

10. A. H. Reshak, S. A. Khan: *Thermoelectric properties of a single graphene sheet and its derivatives*. J. Mater. Chem. C, 2 (2014) 2346.
11. A. H. Reshak, S. A. Khan: *Linear and nonlinear optical properties for AA and AB stacking of carbon nitride polymorph (C3N4)*. RSC Adv. 4 (2014), 11967.
12. A. H. Reshak, S. A. Khan, *Investigation of electronic structure and optical properties of* $MgAl_2O_4$*: DFT approach*. Opt. Mater. 37 (2014) 322.
13. H. Ud Din, S. Azam S. A. Khan, R. Khenata: *Optoelectronic behavior of Quaternary Uranium Chalcogenides* $Rb_2Pd_3UM_6(M = S, Se)$*: A first principle study*. J. Alloys Compd. 615 (2014) 507.
14. A. H. Reshak, Y. Al-Douri, R. Khenata, W. Khan, S. A. Khan, S. Azam: *Electronic structure, Fermi surface topology and spectroscopic optical properties of* $LaBaCo_2O_{5.5}$ *compound*. J. Magn. Magn. Mater. 363(2014)
    133.
15. S. Azam, S. A. Khan, F. A. Shah, S. Muhammad, H. Ud Din, R. Khenata: *Electronic, optical and thermoelectric properties of* Ce_3PdIn_{11} *and* $Ce_5Pd_2In_{19}$ *: An ab initio study*. Intermetallics 55 (2014) 184.
16. S. A. Khan, A. H. Reshak: *Linear, nonlinear optical susceptibilities, hyperpolarizability, and space electronic charge density of meso silver(I) histidinate [Ag(D-his)]n (Hhis = histidine)*. Polyhedron 85 (2015) 962.
17. A. H. Reshak, S. A. Khan: *First principle investigation of electronic structure and optical behaviors of 2-amino-4-fluorododec-4-encarbolic acid*. Mater. Sci. Semicond. Process. 31 (2015) 302.
18. M. Ullah, S. A. Khan, G. Murtaza, R. Khenata, N. Ullah, S. Bin Omran: *Electronic, thermoelectric and magnetic properties of* La_2NiMnO_6 *and* La_2CoMnO_6. J. Magn. Magn. Mater. 377(2015)197.
19. S. A. Khan, S. Azam: *First principle investigation of electronic structure, chemical bonding and optical properties of tetrabarium gallium trinitride oxide single crystal*. Mater. Res. Bull. 70 (2015) 436.
20. S. A. Khan, S. Azam, F. A. Shah, B. Amin: *Electronic structure and optical properties of CdO from bulk to nanosheet: DFT approach*. Opt. Mater. 47 (2015) 372.
21. S. Azam, S. A. Khan, S. Goumri-Said: *Exploring the electronic structure and optical properties of the quaternary selenide compound,* $Ba_4Ga_4SnSe_{12}$*: For photovoltaic applications*. J. Solid State Chem. 229 (2015) 260.
22. A. Bendjedid, T. Seddik, R. Khenata, H. Baltache, G. Murtaza, A. Bouhemadou, S. Bin Omran, S. Azam, S. A. Khan: *GGA+U study on phase transition, optoelectronic and magnetic properties of* AmO_2 *with spin-orbit coupling*. J. Magn. Magn. Mater. 396 (2015) 190.

23. S. Azam, S. A. Khan, R. Khenata, G. Murtaza, S. Bin Omran, S. Muhammad: *Optoelectronic and Magnetic Properties of $Eu_2Si_5N_8$: An Ab-initio Study.* Zeitschrift für Naturforschung A, 70 (2015) 187.
24. S. Azam, S. A. Khan, S. Goumri-Said: *Engle-Vosko GGA Approach Within DFT Investigations of the Optoelectronic Structure of the Metal Chalcogenide Semiconductor $CsAgGa_2Se_4$.* J. Electron. Mater. 45 (2015) 1.
25. S. Azam, S. A. Khan, S. Goumri-Said: *Modified Becke-Johnson (mBJ) exchange potential investigations of the optoelectronic structure of the quaternary diamond-like semiconductors Li_2CdGeS_4 and Li_2CdSnS_4.* Mater. Sci. Semicond. Process. 39 (2015) 606.
26. S. Azam, S. A. Khan, W. Khan, S. Muhammad, H. Udin, G. Murtaza, R. Khenata, F. A. Shah, J. Minar, W. K. Ahmed: *Detailed DFT studies of the electronic structure and optical properties of $KBaMSe_3$ ($M = As, Sb$).* J. Alloys Compd. 644 (2015) 91.
27. S. Azam, S. A. Khan, J. Minar, S. Goumri-Said: *Exploring the electronic structure and optical properties of new inorganic luminescent materials $Ba(Si, Al)_5(O, N)_8$ compounds for light-emitting diodes devices.* Curr. Appl. Phys. 15 (2015) 1160.
28. S. Azam, S. A. Khan, S. Goumri-Said: *Revealing the optoelectronic and thermoelectric properties of the Zintl quaternary Arsenides $ACdGeAs_2$ ($A = K, Rb$).* Mater. Res. Bull. 70 (2015) 847.
29. S. Azam, S. A. Khan: *A first principles study of electronic and optical properties of the polar quaternary chalcogenides $\beta - A_2Hg_3Ge_2S_8$ ($A = KandRb$).* Mater. Sci. Semicond. Process. 34 (2015) 250.
30. F. A. Shah, S. A. Khan, S. Arif, S. Azam, R. Khenata, S. Bin-Omran: *Theoretical investigation of electronic structure and optical response and their interrelation with the transport properties of $Ga_{1-x}In_xN(x = 0, 0.25, 0.50, 0.75)$.* Curr. Appl. Phys. 15 (2015) 608.
31. S. Azam, S. A. Khan, J. Minar, W. Khan, H. Ud Din, R. Khenata, G. Murtaza, S. Bin-Omran, S. Goumri-Said: *Coulomb interaction and Spin-orbit coupling calculations of thermoelectric properties of the quaternary chalcogenides $Tl_2PbXY_4(X = Zr, HfandY = S, Se)$.* Semicond. Sci. Technol. 30 (2015) 105018.
32. M. Faizan, G. Murtaza, S. Azam, S. A. Khan, A. Mahmood, A. Yar: *Elastic and optoelectronic properties of novel Ag_3AuSe_2 and Ag_3AuTe_2 semiconductors.* Mater. Sci. Semicond. Process. 52 (2016) 8.
33. S. Azam, S. A. Khan, H. Ud Din, R. Khenata, S. Goumri-Said: *Exploring the thermoelectric and magnetic properties of uranium selenides: $Tl_2Ag_2USe_4$ and $Tl_3Cu_4USe_6$.* J. Magn. Magn. Mater. 413 (2016) 57.
34. S. Azam, S. A. Khan, S. Goumri-Said: *DFT combined to Boltzmann transport theory for optoelectronic and thermoelectric properties investigations for monoclinic metallic selenide: $Cu_5Sn_2Se_7$.* Optik 127 (2016) 5472.

35. A. Basit, S. A. Khan, G. Murtaza, A. Mehmood, R. Khenata, S. Bin Omran, M. Yaseen: *Electronic, optical and thermoelectric properties of* $XNMg_3(X = P, As, Sb, Bi)$ *compounds.* Mater. Sci. Semicond. Process. 43 (2016) 69.

36. S. A. Khan, S. Azam, O. Sipr:*Interrelationship between structural, optical and transport properties of* $InP_{1-x}Bi_x$*: DFT approach.* Mater. Sci. Semicond. Process. 41 (2016) 45.

37. K. C. Bhamu, R. Khenanta, S. A. Khan, M. Singh, K. R. Priolkar: *Electronic, Optical and Thermoelectric Properties of* $2H - CuAlO_2$*: A First Principles Study.* J. Electron. Mater. 45 (2016) 615.

38. A. Basit, G. Murtaza, A. Mahmood, S. A. Khan, M. Aneel, A. Yar, K. M. Wong: *Specific features investigation of the* AE_2ZnN_2 *(AE=Ca, Sr, Ba) compounds from indirect to direct band gap: DFT study* Mater. Sci. Semicond. Process. 57 (2017) 116.

39. S. Azam, S. A. Khan, S. Goumri-Said: *DFT study of optoelectronic and magnetic properties of iron containing diamond-like materials* Ag_2FeSiS_4*,* $Li2FeSnS_4$*, and* Li_2FeGeS_4 Solid State Sci. 72 (2017) 71.

40. T. Seddik, G. Ugur, F. Soyalp, R. Khenata , D. Prakash, I.V. Kityk, S. A. Khan, A. Bouhemadou, S. Bin-Omran, D. P. Rai, K.D. Verma: *Computational investigations on band structure and electronic features of chromium-based carbides and nitride* Cr_3PX *(X= C and N) through the FP-APW+LO approach* Superlattices Microstruct. 109 (2017) 1.

41. S. Azam, S. A. Khan and S. Goumri-Said: *Exploring the optoelectronic properties of Nitridomagneso-silicates:* $Ca[Mg_3SiN_4]$*,* $Sr[Mg_3SiN_4]$*, and* $Eu[Mg_3SiN_4]$ Semicond. Sci. Technol. 32 (2017) 055017.

42. S. Azam, S. A. Khan, S. Goumri-Said and M. Benali Kanoun, *Predicted Thermoelectric Properties of the Layered* XBi_4S_7 *(X = Mn, Fe) Based Materials: First Principles Calculations* J. Electron. Mater. 46 (2017) 23.

43. M. Ullah, G. Murtaza, M. Yaseen, S. A. Khan:*Band structure features, chemical bonding and optical properties of* Zn_3X2 *(X= N, P, As) compounds* J. Alloys Compd. 728 (2017) 1226.

44. I. Hatraf, O. Merabiha, T. Seddik, H. Baltache, R. Khenata, R. Ahmaed, S. A. Khan, A. Bouhemadou, S. Azam and S. Bin Omran, Bull. Mater. Sci. 40 (2017) 1105.

45. S. Azam, S. A. Khan, and S. Goumri-Said*Polymorph phosphor* $SrSi_2O_2N_2$*:*Eu_{2+} *optoelectronic properties for highly efficient LED: ab-initio calculations* Mater. Today Commun. (2017) DOI : 10.1016/j.mtcomm.2017.10.003

46. S. A. Khan, S. Azam, M. B. Kanoun, G. Murtaza, M. Rani, S. Goumri-Said: *Tailoring the electronic structure and optical properties of cadmium doped Zinc oxides nanosheet* Cogent Physics 4 (2017) 1391734.

47. M. Irfan, S. Hussain, S. A. Khan, S. Goumri-Said, S. Azam:*Optoelectronic Structure and Related Transport Properties of* $Ag_2Sb_2O_6$ *and* $Cd_2Sb_2O_7$ J. Electronic Mater. 47 (2018) 1481.

48. M. Irfan, S. Hussain, S. A. Khan, S. Azam, S. Goumri-Said:*Investigations of Fermi Surface and Optoelectronic Properties of Pyrochlore Oxide Superconductor (KOs2O6): GGA+U+SOC and DFT* J. Phys. Res. Appl. 1 (2018) 1.
49. S. Azam, S. A. Khan, S. Goumri-Said:*Optoelectronic and Thermoelectric Properties of Bi_2OX_2 (X = S, Se, Te) for Solar Cells and Thermoelectric Devices* J. Elec. Mater 47 (2018) 2513.
50. S. Azam, S. Hussain, S. A. Khan, M. Suhail, M. Ahmad, S. Goumri-Said:*Enhanced thermoelectric properties of $ASbO_3$ due to decreased band gap through modified becke and johnson potential scheme* J. Phys. Chem. Solids 119 (2018) 85.
51. M. Irfan, S. A. Khan, S. Azam, M. Rani, I. Kityk, Z. Abbas:*Effects of compressed strain on thermoelectric properties of Cu_3SbSe_4* J. Alloys Compd. 750 (2018) 804.
52. M. Irfan, S. Azam, S. Hussain, S. A. Khan, M. Sohail, M. Makhdoom, Z. Ali, I.V. Kityk, S. Muhammad, A. G. Al-Sehemi:*Effect of Coulomb interactions on optoelectronic and magnetic properties of novel $A_2V_2O_7$ (A= Fe and Co) compounds* J. Alloys Compd. 766 (2018) 536.
53. S. A. Khan and S. Azam:*Electronic structure and thermoelectric properties of $PbS_{1-x}Te_x$ (x=0, 0.25, 0.50, 0.75, 1.0) alloys: ab initio study* Superlattices and Microstructures, 124 (2018) 248.
54. I. Ahmad and S. Ali Khan and M. Idrees and M. Haneef and I. Shahid and H. Ud Din, S. A. Khan and B. Amin:*Influence of strain on specific features of MoX_2 (X = S, Se, Te) monolayers* Physica B: Condensed Matter 545 (2018) 113.
55. S. Azam and M. Irfan and S. A. Khan and Z. Ali and I.V. Kityk and S. Muhammad and A. G. Al-Sehemi:*Doping induced effect on optical and band structure properties of $Sr_2Si_5N_8$ based phosphors: DFT approach* J. Alloys Compd. 771 (2019) 1072.
56. N. Serir, F. Ckiker, H. Khachai, A. Bouhemadou, Saleem Ayaz Khan, T. Ouahrani, Sikander Azam, S.H. Naqib, Ajaya K. Singh, R. Khenata:*Electronic, elastic, thermodynamic and vibrational properties of Li6BeZrF12: Insights from DFT-based computer simulation* Computational Condensed Matter, 25 (2020) 00506
57. S. Azam, M. Irfan, Z. Abbas, S. A. Khan, R. Khenata, S. Muhammad, S. M. Siddeeg, S.H. Naqib, X. Wang:*Optoelectronic properties of Nd^{3+} doped CaTa2O6: Insights from the GGA+U calculations* Optik (2020) 165270.
58. M. Ghazanfar, S. Azam, M. F. Nasir, S. A. Khan, Hafiz Usama, M. Irfan, S. Muhammad, A. G. Al-Sehemi, S.H. Naqib, R. Khenata, S. Goumri-Said, X.T. Wang:*Exploring the potential use of Ca[LiAl3N4]:Eu^{2+} as phosphor-LED material: Ab-initio calculations* Materials Today Communications, 25 (2020) 101302.
59. M. Iqbal, J. Fatheema, Q. Noor, M. Rani, M. Mumtaz, Ren-Kui Zheng, S. A. Khan, S.Rizwan:*Co-existence of magnetic phases in two-dimensional MXene* Materials Today Chemistry16 (2020) 100271.
60. S. Azam, S. Goumri-Said, S. A. Khan, H. Ozisik, E. Deligoz, M. B. Kanoun, W. Khan:*Electronic structure and related optical, thermoelectric and dynamical properties of Lilianite-type Pb7Bi4Se13:*

Ab-initio and Boltzmann transport theory Materialia 10 (2020) 100658.

61. A. Mahmood, S. Azam, M. Irfan, M. A. Kamran, T. Alharbi, A. Majid, M. W. Iqbal, S. Muhammad, A. G. Al-Sehemi, S. A. Khan, S. Goumri-Said: *Cation effect on electronic, optical and thermoelectric properties of perovskite oxynitrides: Density functional theory* Materials Science in Semiconductor Processing, 107 (2020) 104800.