# SHAKEEL AHMAD KHANDY

**D.O.B:** 02-April-1990
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## PRESENT AFFILIATION:

Frontier Research Institute for Interdisciplinary Sciences
Islamic University of Science and Technology,
Awantipora-192122 J&K-India
**(Ramanajun Fellow/Scientist-D)**
April. 2024 to till date

## PROFILE

I am interested in studying the electronic structure and other physical properties of novel and multifunctional materials. Currently, I am working on the design of new 2D-materials and Nano-layers for possible energy harvesting applications.

## EXPERTISE

WIEN2k, BoltzTrap, VASP, Quantum Espresso, etc.

**Citations: 1960; h-index: 28; i10-index: 45**

**Research Gate:**
https://www.researchgate.net/profile/Shakeel_Khandy
**Google Scholar:**
https://scholar.google.co.in/citations?user=UmKxJkcAAAAJ&hl=en

**Scopus Author ID:** 57189444970
**Researcher ID:** AAE-6879-2019
**Loop profile:** 906646

## SELECTED PUBLICATIONS:

- ***Journal of Physics Chemistry Letters*** (2023) *14, 21, 5004-5012*.
- ***Materials Chemistry and Physics*** 296 (2023) 127293
- ***Molecules*** 27 (2022) 3785.
- ***Journal of Physics and Chemistry of Solids*** 165 (2022) 110649
- ***Scientific Reports***, 11 (2021) 20756.
- ***Journal of Alloys and Compounds*** 850 (2021) 156615
- ***Nanoscale***, 12 (2020) 16910.
- ***Journal of Applied Physics*** 127 (2020) 165102.
- ***Scientific Reports*** 9 (2019) 1475.
- ***Journal of Magnetism and Magnetic Materials***, 487, (2019) 165289.
- ***International Journal of Energy Research***, 42(13) (2018).
- ***RSC Advances***, 8 (2018) 40996
- ***Semiconductor Science and Technology***, 32 (2017) 125019
- ***Journal of Magnetism and Magnetic Materials***, 441 (2017) 166.
- ***RSC Advances***, 6 (2016) 97641
- ***RSC Advances***, 6 (2016) 48009

## EXPERIENCE:

- Zhejiang University, Hangzhou-310027, China. **(Pos.Doc.)**
  Nov. 2021 to March 2024
  Advisors: **Prof. Bin Yu & Dr. Hua Wang**
- National Taiwan University, Taipei-106319, Taiwan. **(Pos.Doc.)**
  Dec. 2018-Oct. 2021
  Advisor **Prof. Jeng Da- Chai**
- Islamic University of Science and Technology, Awantipora-192122 J&K-India (**Asst. Professor**)
  April 2018 to Nov 2018
- Indian Institute of Technology Madras-Chennai, 600036-India. **(Pos.Doc.)**
  Dec. 2017 to March 2018
  Advisor. **Prof. B.R.K. Nanda**

## EDUCATION:

**Ph.D. Physics:** Jiwaji University Gwalior (MP), INDIA-474011
(28-March-2015 to 23-Sep-2017)
[*ab-initio* Study of Magnetism and Electronic Properties of Some Perovskites]
Advisor. **Prof. Dinesh C Gupta**
**Master's Physics:** Jiwaji University Gwalior (MP), INDIA-474011
(July-2011 to June-2013)

## AWARDS AND FELLOWSHIPS:

- **2024** Ramanujan Fellowship by DST-SERB Govt. of India
- **2023** Top **2% scientists** (https://mp.weixin.qq.com/s/NW_VdfSCIRm-HLrNI8V_Mw)
- **2023** Hangzhou High-level Talent Classification Certificate (**E-Talent**)
- **2022-2024** High-Talent Research Fellowship from Hangzhou Global Scientific and Technological Innovation Center, Zhejiang University (ZJU), Hanghzhou, China
- **2022** Top **2% Scientists** (https://doi.org/10.17632/btchxktzyw.4)
- **2019-2021** Taiwan Post-Doctoral fellowship from National Taiwan University-Taipei, Taiwan (ROC).
- **2019**-Selected for Paper Presentation and Travel Grant, ICTP, Italy.
- **2018**-Awarded Post Doctorial fellowship by International Centre for Quantum & Molecular Structures Department of Physics Shanghai University, China. (N/A)
- **2018**-Awarded RA/PDF fellowship by Department of Physics, IIT Madras (Chennai) India.
- **2017**-Awarded PDF by Natural Sciences (Molecular Quantum Dynamics and Information Theory (M-QuDIT), Sungkyunkwan University (Seoul), South Korea. (N/A)
- **2017**-Meritorious University Fellowship Award, Jiwaji University Gwalior.
- **2016**-Young Scientist Training and Fellowship Award, M.P Council of Science & Technology-Bhopal.

## COLLABORATIONS:

- Zhejiang University, Hangzhou-310027, China.
- Southwest University, Chongqing 400715, China
- University of Bremen, Leobener Strasse 7, Bremen 28359, Germany
- National Taiwan University of Science and Technology 106335, Taiwan
- King Saud University, Riyadh 11415, Saudi Arabia
- Université de Mascara, Mascara 29000, Algeria

## REFERENCES:

Will be provided on request

**Shakeel**

## Peer-Reviewed Publications

1. M.A. Ali, A.A. Alothman, S. Mohammad, A. Khan, **Shakeel Ahmad Khandy** & M. Faizan, *State of Art in Lead Free Double Perovskite Ceramics, $X_2MgTeO_6$(X = Sr, Ba): Structural Stability and their Potential Energy harvesting Applications.* **Journal of Inorganic and Organometallic Polymers and Materials** -- (2024) -- https://doi.org/10.1007/s10904-024-03115-2
2. M.A. Ali, A. Khan, R.A. Alshgari, S. Mohammad and **Shakeel Ahmad Khandy**, *A theoretical study of stable direct band gap double perovskites $X_2YIO_6$ (X = K, Rb) for renewable energy applications.* **Optical and Quantum Electronics** 56 (2024) 931 https://doi.org/10.1007/s11082-024-06917-3
3. B. Kaur, Heena, **Shakeel Ahmad Khandy***, S.R. Ahmad, M.D Albaqami, M. Srinivasan, L. Patra, S. Dhiman and, K. Kaur* *Thermoelectric Properties of 2D$Sn_2SSe$ Monolayer,* **Advanced Quantum Technologies** -- (2024) -- https://doi.org/10.1002/qute.202300357
4. Y. Seksak, R. Moussa*, M. Boudjelal, R. Khenata*, A. Abdiche, W.K. Ahmed, **Shakeel Ahmad Khandy***, A. Bouhemadou and S. Bin-Omran. *An in-depth look at the structural, electronic, optical, and thermal properties of the cubic $Be_xMgyZn_{1-x-y}O$ quaternary alloys,* **Physica Scripta** 99 (2024) 045945 https://doi.org/10.1088/1402-4896/ad3173
5. **Shakeel Ahmad Khandy***, I. Islam, K. Kaur, A.M. Ali, M.A. Sayed and, K. Kaur *Strain dependent electronic structure, phonon and thermoelectric properties of CuLiX (X=S,Te) Half Heusler compounds,* **Physica B: Condensed Matter** 677 (2024) 415698 https://doi.org/10.1016/j.physb.2024.415698
6. N. Mehak, B. Rani, A.F. Wani, **Shakeel Ahmad Khandy***, A.S. Verma, A.M. Ali, M.A. Sayed, S. Dhiman and K. Kaur*, First principle examination of two-dimensional rare-earth metal germanide halides $Y_2GeX_2$ (X = Cl, Br, I) for thermoelectric applications, **Materials Science in Semiconductor Processing** 171 (2024) 107995. https://doi.org/10.1016/j.mssp.2023.107995
7. A.F. Wani, **Shakeel Ahmad Khandy***, I. Islam, A.M. Ali, S. Dhiman and K. Kaur*, Intrinsic and strain dependent ultralow thermal conductivity in novel AuX (X = Cu, Ag) monolayers for outstanding thermoelectric applications, **Physical Chemistry Chemical Physics** 25 (2023) 21736-21747. https://doi.org/10.1039/D3CP01038D
8. B. Rani, **Shakeel Ahmad Khandy***, J. Singh, A.S. Verma, A.M. Ali, S. Dhiman and K. Kaur, Electronic structure, elastic and transport properties of new Palladium-based Half-Heusler Materials for Thermoelectric Applications, **Materials Today Communications** 36 (2023), 106461. https://doi.org/10.1016/j.mtcomm.2023.106461
9. A.A. Bhat, I. Assadullah, A. Farooq, K.A. Malik, J.H. Malik, R. Tomar, I Islam, A.M. Ali and **Shakeel Ahmad Khandy***, Band-gap alteration of $Zn_2SnO_4$ nanostructures for optical and photo-luminescent applications, **Materials Chemistry Physics** 306 (2023) 127993. https://doi.org/10.1016/j.matchemphys.2023.127993

10. A.A. Bhat, **Shakeel Ahmad Khandy***, A.M. Ali and R.Tomar, Photoluminescence Emission Studies on a Lanthanum-Doped Lead Free Double Halide Perovskite, La:$Cs_2SnCl_6$, **Journal of Physics Chemistry Letters** 14(21) (2023) 5004-5012. https://doi.org/10.1021/acs.jpclett.3c00522
11. J. Singh, T. Kaur, A.P. Singh, M. Goyal, K. Kaur, **Shakeel Ahmad Khandy**, I. Islam, A.F. Wani, R. Krishan, M.M. Sinha and S.S. Verma, LiNbCoX (X = Al, Ga) quaternary Heusler compounds for high-temperature thermoelectric properties: a computational approach, **Bulletin of Materials Science** 46 (2) (2023) 1-13. https://doi.org/10.1007/s12034-023-02945-z
12. J. Singh, K. Kaur, I. Islam, J.M. Mir, M. Goyal, T. Kaur, SS Verma, A.M. Ali and **Shakeel Ahmad Khandy***, Electronic structure, phonon stability, mechanical and high-temperature thermoelectric properties of Li-based quaternary Heusler alloys, **Current Applied Physics** 50 (2023) 161–167. https://doi.org/10.1016/j.cap.2023.04.010
13. **Shakeel Ahmad Khandy***, I. Islam, K. Kaur, A.M. Ali, and A.F. Abd El-Rehim, Electronic structure, stability, photocatalytic and optical properties of new lead-free double perovskites $Tl_2PtX_6$ (X = Cl, Br) for light-harvesting applications, **Materials Chemistry and Physics** 296 (2023) 127293. https://doi.org/10.1016/j.matchemphys.2023.127293
14. Javied Hamid Malik, Khurshaid Ahmad Malik, Insaaf Assadullah, Adil Ahmad Bhat, Ishtihadah Islam, Vipin Shrotriya, M Burhanuz Zaman, Radha Tomar, **Shakeel Ahmad Khandy***, Electronic structure, growth and properties of hydrothermally derived crystalline $Cu_2MnSnS_4$ quantum dots: optimization of physiochemical parameters and electrochemical performance, **Applied Physics A** 129 (2023) 86. https://doi.org/10.1007/s00339-022-06369-0
15. B. Rani, A.F. Wani, U.B. Sharapov, L. Patra, J. Singh, A.M. Ali, A.F. Abd El-Rehim, **Shakeel Ahmad Khandy***, S. Dhiman, and K. Kaur, Electronic Structure, Phonon Spectrum, and Effective Mass- Related Thermoelectric Properties of PdXSn(X= Zr, Hf) Half Heuslers, **Molecules** 27(19) (2022) 6567. https://doi.org/10.3390/molecules27196567
16. T. Kaur, J. Singh, M. Goyal, K. Kaur, **Shakeel Ahmad Khandy**, M.A. Bhat, U. Sharopov, S. Dhiman, A.F. Wani, B. Rani, M.M. Sinha and S.S. Verma, First principles calculations to investigate Li-based quaternary Heusler compounds LiHfCoX (X= Ge, Sn) for thermoelectric applications, ***Physics Scripta*** 97 (2022) 105706. https://doi.org/10.1088/1402-4896/ac8c70
17. J. Singh, K. Kaur, M.A. Bhat, U.B. Sharopov, S. Dhiman, M. Goyal, S.S. Verma, **Shakeel Ahmad Khandy***, First-principles calculations on the electronic structure and thermoelectric properties of quaternary Heusler compounds: LiScPtSi and LiScPdGe, ***Materials Today Communications*** 32 (2022) 103961. https://doi.org/10.1016/j.mtcomm.2022.103961
18. **Shakeel Ahmad Khandy***, I. Islam, K. Kaur, A.M. Ali, and A.F. Abd El-Rehim, Effect of Strain on the Electronic Structure and Phonon Stability of SrBaSn Half Heusler Alloy, ***Molecules*** 27 (2022) 3785. https://doi.org/10.3390/molecules27123785

19. B. Rani, A.F. Wani, **Shakeel Ahmad Khandy**, U. Sharopov, L. Patra, K. Kaur, S. Dhiman, Pursuit of stability, electronic and thermoelectric properties of novel PdVGa half heusler compound, ***Solid State Communications*** 351 (2022) 1147964. https://doi.org/10.1016/j.ssc.2022.114796
20. K. Kaur, **Shakeel Ahmad Khandy***, S. Dhiman, U. Sharopov, J. Singh, Computational prediction of thermoelectric properties of 2D materials, ***Electronic Structure*** 4 (2022) 023001. https://doi.org/10.1088/2516-1075/ac635b
21. I. Assadullah, A.A. Bhat, J.H. Malik, K.A. Malik, R. Tomar, **Shakeel Ahmad Khandy*** Electronic structure, optical, photocatalytic and charge storage performance of $WO_3$ nanostructures, ***Journal of Physics and Chemistry of Solids*** 165 (2022) 110649. https://doi.org/10.1016/j.jpcs.2022.110649
22. S.A. Dar, B. Want, **Shakeel Ahmad Khandy**, Computer based predictions of structural stability and systematic study of magneto-electronic and optical properties of Lead-Free Halide Double Perovskites: $Cs_2KXCl_6$: X = Co and Ni, ***Journal of Magnetism and Magnetic Materials***, 545, (2022) 168603. https://doi.org/10.1016/j.jmmm.2021.168603
23. **Shakeel Ahmad Khandy*** Inspecting the electronic structure and thermoelectric power factor of novel p-type half-Heuslers, ***Scientific Reports*** 11 (2021) 20756. https://www.nature.com/articles/s41598-021-00314-6
24. M. Benidris, Z. Aziz, A. Bennani, M. Matougui, S. Terkhi, M. Houari, B. Bouadjemi, **Shakeel Ahmad Khandy** High dimensionless figure of merit in full Heusler alloy Ru2ZrSi: A first principles study, ***Solid State Communications*** (2021) 114466. https://doi.org/10.1016/j.ssc.2021.114466
25. M.A. Boudjeltia, Z. Aziz, S. Terkhi, M.A. Bennani, **Shakeel Ahmad Khandy,** B. Bouadjemi, M. Benidris and S. Bentata, Theoretical investigation of ternary semiconductors half-Heusler RhTaZ (Z = Si, Ge and Sn) for thermoelectric applications, ***Modern Physics Letters B*** 35(23) (2021) 2150400. https://doi.org/10.1142/S0217984921504005
26. A. Bhat, **Shakeel Ahmad Khandy*,** I. Islam and R. Tomar, Optical, electrochemical and photocatalytic properties of cobalt doped $CsPbCl_3$ nanostructures: A one-pot synthesis approach, ***Scientific Reports*** 11 (2021) 16473. https://doi.org/10.1038/s41598-021-95088-2
27. M. Benidris, Z. Aziz, **Shakeel Ahmad Khandy**, S. Terkhi, M.A. Ahmad, B. Bouadjemi, M.A. Bennani and A. Laref, Electronic structure, thermoelectric, mechanical and phonon properties of full-Heusler alloy ($Fe_2CrSb$): A first-principles study, ***Bulletin of Material Science*** 44 (2021) 221. https://doi.org/10.1007/s12034-021-02496-1
28. J. Singh, K. Kaur, **Shakeel Ahmad Khandy***, S. Dhiman, M. Goyal and S S Verma, Structural, electronic, mechanical, and thermoelectric properties of LiTiCoX (X = Si, Ge) compounds, ***International Journal of Energy Research*** 45 (2021) 1689. https://doi.org/10.1002/er.6851
29. **Shakeel Ahmad Khandy** and J.D. Chai, Origin of pseudo gap and thermoelectric signatures of semimetallic $Ru_2TaGa$: Structural stability from phonon dynamics, mechanical and thermodynamic predictions, mechanical and thermodynamic prediction, ***Journal of Physics and Chemistry of Solids*** 154 (2021) 110098. https://doi.org/10.1016/j.jpcs.2021.110098

30. M.B. Zaman, P. Rajaram, **Shakeel Ahmad Khandy**, A. Modi and R.K. Tiwari, Thioglycolic acid assisted hydrothermal growth of SnS 2D nanosheets as catalysts for photodegradation of industrial dyes, ***Nanotechnology*** 32 (2021) 245706. https://doi.org/10.1088/1361-6528/abec09
31. **Shakeel Ahmad Khandy***, S.A. Vaid, I. Islam, A.K. Hafiz and J.D. Chai, Understanding the stability concerns and electronic structure of $CsYbX_3$ (X=Cl,Br) halidoperovskites for optoelectronic applications, ***Journal of Alloys and Compounds*** 867 (2021) 158966. https://doi.org/10.1016/j.jallcom.2021.158966
32. I. Islam, **Shakeel Ahmad Khandy***, M.B. Zaman, AK. Hafiz, A.M. Siddiqui and J.D. Chai, Growth and characterization of crystalline $BaSnO_3$ perovskite nanostructures and the influence of heavy Mn doping on its properties, ***Journal of Alloys and Compounds*** 867 (2021) 158900. https://doi.org/10.1016/j.jallcom.2021.158900
33. **Shakeel Ahmad Khandy*,** K. Kaur, S. Dhiman, J. Singh and V. Kumar, Exploring thermoelectric properties and stability of half-Heusler PtXSn (X = Zr, Hf) semiconductors: *A first principle investigation*, ***Computational Material Science*** 188 (2021) 110232. https://doi.org/10.1016/j.commatsci.2020.110232
34. **Shakeel Ahmad Khandy** and J.D. Chai, Strain engineering of electronic structure, phonon, and thermoelectric properties of p-type half-Heusler semiconductor, ***Journal of Alloys and Compounds*** 850 (2021) 156615. https://doi.org/10.1016/j.jallcom.2020.156615
35. X. Wang, G. Ding, **Shakeel Ahmad Khandy#**, Z. Chen, G. Zhang, X.-L. Wang and H. Chen, Unique topological nodal line states and associated exceptional thermoelectric power factor platform in $Nb_3GeTe_6$ monolayer and bulk, ***Nanoscale***, 12 (2020) 16910. (#=Equal author) https://doi.org/10.1039/D0NR03704D
36. **Shakeel Ahmad Khandy** and J.D. Chai, Electronic Structure, Magnetism and Mechanical Properties of newly synthesized FeRhCrZ Alloys, ***Journal of Applied Physics*** 127 (2020) 165102. https://doi.org/10.1063/1.5139072
37. **Shakeel Ahmad Khandy***, I. Islam, K. Kaur, A. Laref, S. Dhiman, S. Rubab, D.C. Gupta, R. Khenata, DFT investigations on the electronic structure, magnetism, thermodynamic and elastic properties of newly predicted cobalt based antiperovskites: $Co_3XN$ (X=Pd, Pt & Rh), ***Results in Physics*** 17 (2020) 103112. https://doi.org/10.1016/j.rinp.2020.103112
38. **Shakeel Ahmad Khandy** and J.D. Chai Robust stability, half-metallic ferrimagnetism and thermoelectric properties of new quaternary Heusler material: A first principles approach, ***Journal of Magnetism and Magnetic Materials***, 502, (2020) 166562. https://doi.org/10.1016/j.jmmm.2020.166562
39. A. Laref, R.M. Amer, Z. Alahamad, S. Laref, I. Islam **Shakeel Ahmad Khandy,** Y.C. Xiong, H.M. Haung and X. Wu, Electronic structure and optical anisotropy in $Sr_{1-x}Ba_xFBiS_2$ (x = 0, 0.25, 0.5, 0.75, 1) based solar cell materials, ***Results in Physics*** 16 (2020) 1028082. https://doi.org/10.1016/j.rinp.2019.102808
40. **Shakeel Ahmad Khandy,** I. Islam, K. Kaur, A. Nazir and A. Laref, Electronic structure, magnetism and elastic properties of inverse Perovskite carbide: A first principles study, ***Physica B: Condensed Matter*** 578 (2020) 411839**.** https://doi.org/10.1016/j.physb.2019.411839

41. **Shakeel Ahmad Khandy,** I. Islam, A. Laref, M. Gogolin, A.K. Hafiz and A.M. Siddiqui, Electronic structure, Thermomechanical and Phonon Properties of Inverse Perovskite Oxide ($Na_3OCl$): An ab initio Study, ***International Journal of Energy Research*** 44(4) (2019) 2594. https://doi.org/10.1002/er.4982
42. A. Laref, M. Alsagri, S.M.A. Abbas, S. Laref, H.M. Haung, Y.C. Xiong, J.Yang, **Shakeel Ahmad Khandy,** D. Ray, D. Varshney and X. Wu, Electronic structure and optical properties of AA stacked bilayer graphene: A first principles calculation, ***Optik*** 206 (2020) 163755. https://doi.org/10.1016/j.ijleo.2019.163755
43. M.M. Obeid, M.M. Shukur, S.J. Edrees, R. Khenata, M.A. Ghebouli, **Shakeel Ahmad Khandy**, A Bouhemadou and H.R. Jappor, Electronic Band Structure, Thermodynamics and Optical Characteristics of $BeO_{1-x}A_x$ (A= S, Se, Te) Alloys: Insights from Ab Initio Study, ***Chemical Physics***, 526 (2019) 110414. https://doi.org/10.1016/j.chemphys.2019.110414
44. **Shakeel Ahmad Khandy** and J.D. Chai, Novel half-metallic $L2_1$ structured full-Heusler compound for promising spintronic applications: A DFT-based computer simulation, ***Journal of Magnetism and Magnetic Materials***, 487, (2019) 165289. https://doi.org/10.1016/j.jmmm.2019.165289
45. I. Islam, A.M. Siddiqui, A.K. Hafiz, J. Ali and **Shakeel Ahmad Khandy*** Influence of pH and Fe-doping on structural and physical properties of $Mg_{0.95}Mn_{0.05-x}Fe_xO$ (x=0,0.04) nanoparticles, ***Journal of Physics and Chemistry of solids***, 133, (2019) 197. https://doi.org/10.1016/j.jpcs.2019.05.030
46. L. Boumia, F. Dahmanea, B. Doumi, D.P. Rai, **Shakeel Ahmad Khandy**, H. Khachai, H. Meradji, Ali H. Reshak and R. Khenata, Structural, electronic and magnetic properties of new full Heusler alloys $Rh_2CrZ$ (Z=Al,Ga,In): First-principles calculations, ***Chinese Journal of Physics***, 59 (2019) 281. https://doi.org/10.1016/j.cjph.2019.04.002
47. **Shakeel Ahmad Khandy**, I. Islam, D.C. Gupta R. Khenata and A. Laref, Lattice dynamics, mechanical stability and electronic structure of Fe-based Heusler semiconductors, ***Scientific Reports*** 9 (2019) 1475. https://www.nature.com/articles/s41598-018-37740-y
48. A. Laref, M Alsagri, S. Laref, J.T. Yang, Y.C. Xiong, and **Shakeel Ahmad Khandy**, Relativistic effects on the electronic and optical characteristics of $Cd_{1-x}Hg_xTe$ alloys-based solar cell materials, ***Journal of Physics and Chemistry of Solids*** 129 (2019) 368. https://doi.org/10.1016/j.jpcs.2019.01.033
49. K.A. Parrey, T. Farooq, **Shakeel Ahmad Khandy**, U Farooq and A Gupta, First principle studies on structure, magneto-electronic and elastic properties of photovoltaic semiconductor halide ($RbGeI_3$) and ferromagnetic half metal oxide ($RbDyO_3$), ***Computational Condensed Matter***, 19 (2019) e00381. https://doi.org/10.1016/j.cocom.2019.e00381
50. **Shakeel Ahmad Khandy,** I. Islam, D.C. Gupta and A. Laref, Full Heusler alloys ($Co_2TaSi$ and $Co_2TaGe$) as potential spintronic materials with tunable band profiles, ***Journal of Solid-State Chemistry***, 270 (2019) 173. https://doi.org/10.1016/j.jssc.2018.11.011
51. **Shakeel Ahmad Khandy,** W. Khan, I. Islam, A. Laref, M. Tanveer, D.C. Gupta, S. Rubab and S. Laref, Electronic structure, optical and thermoelectric properties of $CaMgSi_{1-x}C_x$ (x=0,0.5): An ab-initio study, ***Materials Research Express***, 6 (2018) 036307. https://doi.org/10.1088/2053-1591/aaf7d0

52. **Shakeel Ahmad Khandy,** I. Islam, D.C. Gupta, M.A. Bhat, S. Ahmad, T.A. Dar, S. Rubab, S. Dhiman and A. Laref, A case study of $Fe_2TaZ$ (Z=Al,Ga,In) Heusler Alloys: Hunt for Half-metallic behavior and Thermoelectricity, ***RSC Advances***, 8 (2018) 40996. https://doi.org/10.1039/C8RA04433C
53. K.A. Parrey, N. Devi, R. Khenata**, Shakeel Ahmad Khandy,** Investigating structure, magneto-electronic, elastic and thermoelectric properties of alkaline earth actinide perovskite oxide ($BaBkO_3$) from first principle calculations, C***omputational Condensed Matter***, 16 (2018) e00340. https://doi.org/10.1016/j.cocom.2018.e00340
54. **Shakeel Ahmad Khandy,** I. Islam, D.C. Gupta, R. Khenata, A. Laref and Seemin Rubab, First Principles understanding of structural, electronic, elastic and thermal properties of $BaCfO_3$ perovskite, ***Materials Research Express***, 5 (2018) 105702. https://doi.org/10.1088/2053-1591/aad9eb
55. **Shakeel Ahmad Khandy**, I. Islam, D.C. Gupta and A. Laref, Predicting the electronic structure, magnetism and transport properties of new Co-based Heusler alloys, ***International Journal of Energy Research***, 42(13) (2018) 4221. https://doi.org/10.1002/er.4182
56. **Shakeel Ahmad Khandy**, First Principles understanding of Structural Electronic and Magnetic properties of new Quaternary Heusler alloy: FeVRuSi, ***Materials Research Express***, 5 (2018) 056516. https://doi.org/10.1088/2053-1591/aac253
57. **Shakeel Ahmad Khandy**, I. Islam, D.C. Gupta and A. laref, Electronic Structure, Mechanical and Thermodynamic Properties of $BaPaO_3$ under Pressure, ***Journal of Molecular Modelling***, 24 (2018) 131**.** *https://doi.org/10.1007/s00894-018-3666-z*
58. **Shakeel Ahmad Khandy** and D.C. Gupta, Electronic structure, magnetism and Thermoelectric properties of double perovskite $Sr_2HoNbO_6$, ***Journal of Magnetism and Magnetic Materials***, 458 (2018) 176**.** https://doi.org/10.1016/j.jmmm.2018.03.017
59. K.A. Parrey, **Shakeel Ahmad Khandy***, I. Islam, A. Laref, D.C. Gupta, A. Niazi, A. Aziz, S.G. Ansari, R. Khenata and S. Rubab, Electronic Structure, Optical and Transport Properties of Double Perovskite $La_2NbMnO_6$: A Theoretical Understanding from DFT Calculations, ***Journal of Electronic Materials***, 47 (2018) 3615**.** https://doi.org/10.1007/s11664-018-6207-8
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## Conference Proceedings

1. J. Singh, K. Kaur, **Shakeel Ahmad Khandy**, M. Goyal, S. Dhiman, S.S. Verma, Structural, electronic, vibrational, thermoelectric and mechanical properties of Li based quaternary Heusler compound LiTiCoSn: A DFT approach, ***Materials Today: Proceedings*** 57 (2022) 211. https://doi.org/10.1016/j.matpr.2022.02.358
2. J. Singh, K. Kaur, M. Goyal, **Shakeel Ahmad Khandy**, S. Dhiman, and S.S. Verma, Quaternary Heusler Compound LiYNiSn: A Search of New Thermoelectric Material by DFT Study, ***AIP Conf. Proc.*** 2352 (2021) 020028. https://doi.org/10.1063/5.0052372

3. **Shakeel Ahmad Khandy,** I. Islam, T.M. Bhat, S. Yousuf and D.C. Gupta, Structural and electronic properties of half-metallic rare-earth perovskites, ***AIP Conference Proceedings*** 1953 (2018) 110006. https://doi.org/10.1063/1.5033031
4. I. Islam, **Shakeel Ahmad Khandy,** and A.K. Hafiz, Synthesis and Structural Characterization of Transition metal doped MgO: $Mg_{0.94}Mn_{0.01}TM_{0.05}O$ (TM = Co, Ni, Cu), ***AIP Conference Proceedings*** 1953 (2018) 030015. https://doi.org/10.1063/1.5032350
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6. S. Yousuf, **Shakeel Ahmad Khandy**, T.M. Bhat and D.C. Gupta, Evaluation of mechanical and transport properties of $Zr_2CoSi$ Heusler alloy, ***AIP Conference Proceedings*** 1832 (2017) 110005. https://doi.org/10.1063/1.4980629
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## Book Chapters

1. M. Shalaby, S. Hamdy, I. Islam, K. Kaur, A. Nazir, **Shakeel Ahmad Khandy*** Bulk and Nanocomposite Thermoelectrics: Synthesis, Properties, and Applications in **Advances in Nanocomposite Materials for Environmental and Energy Harvesting Applications** by A.E. Shalan, A.S. Makhlouf Hamdy, S. Lanceros-Méndez. (eds). Engineering Materials. Springer, Cham. (**2022**) Pages 959-1016 https://doi.org/10.1007/978-3-030-94319-6_31 (ISBN: 978-3-030-94321-9)
2. K. Kaur, Enamullah, **Shakeel Ahmad Khandy**, J. Singh, S. Dhiman, Traditional thermoelectric materials and challenges, in **Thermoelectricity and Advanced Thermoelectric Materials** Edited by R. Kumar, R. Kumar, Wood head Publishing Series in Electronic and Optical Materials, (**2021**), Pages 139-161. https://doi.org/10.1016/B978-0-12-819984-8.00009-6 (ISBN: 978-0-12-819984-8) Copyright © 2021 Elsevier Ltd. All rights reserved.

## Invited Lectures

2023 Invited talk at 10th International Congress on Industrial and Applied Mathematics 2023 JAPAN (ICIAM2023 @ Tokyo: August 20-25, 2023).

2023 International workshop on Quantum Mechanical Modelling using Quantum Espresso (IWQMMM-2023) organised by IEEE Nanocouncil PSIT-Kanpur Student chapter in association with MRSI Allahabad chapter and School of Basic Science, CSJM University -UP-India

2022 A special lecture on the "Thermoelectric materials and their properties" Department of Physics, Islamic University of Science and Technology (IUST)-Kashmir-India

2019 THE 19th WORKSHOP on FIRST-PRINCIPLES COMPUTATIONAL MATERIALS PHYSICS at National Taiwan University-Taipei Taiwan

2019 Department of Applied Sciences PEC Chandigarh-Deemed University, Chandigarh India.

## Conference Presentations

2019 International Conference on Modern Concepts and New Materials for Thermoelectricity at The Abdus Salam International Centre for Theoretical Physics (ICTP)-Trieste Italy.

2018 Conference on Study of Nanomaterials and Scientific Development in 21st Century (ICSNSDC) and IVth Annual Meeting of "Academy of Microscope Science & Technology (AMST), India at Jiwaji University, Gwalior.

2017 International Conference on Recent Trends in Chemical Science (ICRCS-17) at Govt. Engineering College, Bikaner Rajasthan India.

2016 Seminar on Recent Trends in Current Research and its Benefits to Society at Jiwaji University, Gwalior.

2016 International conference on Nanotechnology for better living at National Institute of Technology Srinagar, Jammu and Kashmir.

2015 National conference on scientific developments in 21st century, at Jiwaji University, Gwalior.