

**Dr. Rana Muhammad Arif Khalil**

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Associate Professor, Institute of Physics,  
Bahauddin Zakariya University, Multan.

H Index :31 as per Web of Science

Top 2% Scientists, Stanford/Elsevier List 2025 Ranked 154325.

**PhD DISSERTATION TITLE:**

“*Ab-initio* Studies of the Structural, Dynamical and Thermodynamical Properties of Graphitic and Hydrogenated Graphitic Materials and their Potential for use in hydrogen storage” supervised by Professor Ian Morrison, Director of Physics, University of Salford, Greater Manchester, UK.

**MEMBERSHIP OF ORGANIZATIONS:**

- Life member of “The Pakistan Institute of Physics (PIP)”.
- Life Member of the Zakariyan Alumni Association of Physicists (ZAAP).

**COURSES TAUGHT TO BS/M.Phil/PhD LEVEL CLASSES:**

Electricity and Magnetism, Solid State Physics, Mechanics, Quantum Mechanics, Conduction in Solids, Waves and Oscillations, Material Science, Dielectric Properties of Materials, Structural Analysis and Crystallography, Mathematical Methods of Physics, Nuclear Physics, Computational Physics, Heat and Thermodynamics.

**ADMINISTRATIVE RESPONSIBILITIES:**

1. Member Board of Studies, University of Okara, Okara
2. Member Board of Studies, Institute of Physics, BZU Multan.
3. Member Admission Committee, Department of Physics, B.Z. University, Multan from July, 2017 to date.
4. Deputy Director of Student Affairs Department of Physics, B.Z. University, Multan.
5. Stock Taking of Teaching and Research Laboratories.
6. Assistance in Curriculum Development for Undergraduate and Postgraduate Level Courses.

**CONFERENCES/ WORKSHOPS/ MEETINGS ATTENDED:**

1. Attended International Conference-2006 organized by Pakistan Institute of Physics UET Lahore in March 13-16, 2006.
2. Attended 1<sup>st</sup> meeting of Nobel Laureates with Pakistani students/Young Scholars in Islamabad from 27-28 March 2006.
3. Participated in the International School on “Surface, Thin Films, Nanostructures and Applications” COMSATS Lahore Oct 27-Nov 01 2006.

4. Attended 58<sup>th</sup> Nobel Laureates meeting held at Lindau ,Germany (June 29<sup>th</sup> to July 4<sup>th</sup> 2008)
5. R. M. A. Khalil and I. Morrison, oral presentation, titled “Atomistic Studies of Radiation Damage in Silicon Carbide” 1<sup>st</sup> CSE Conference at University of Salford, UK November 17, 2010. ISBN: 978-1-905732-0.
6. R. M. A. Khalil and I. Morrison, CASTEP Workshop, Poster Presentation entitled “Structural and Dynamical Properties of Graphite incorporating Dispersion Correction” University of Oxford, UK, August 19-23, 2013.
7. R. M. A. Khalil and I. Morrison, oral presentation, titled “Structural and Dynamical Studies of Graphitic Materials” 4<sup>th</sup> CSE Doctoral School Postgraduate Conference, Salford, UK, November 13, 2013. ISBN: 978-1-907842-50-4.
8. R. M. A. Khalil and I. Morrison, Poster Presentation entitled “An Accurate Dispersion Corrected Studies of Structural and Vibrational Properties of Graphite” Dean’s Annual Research Show Case Salford, UK June 18, 2014.
9. Participated in National workshop on Physics Education, Challenges & Prospects, NCP Islamabad November 26-27, 2015.
10. COMSTECH-CIIT Joint International Workshop on Rational Design of Materials for Energy Needs: Computation and Experimentation, COMSTECH Islamabad, Pakistan May 22-26, 2017.
11. Participated to organize Seminar on EU Research and Innovation Programme, Horizon 2020, Bahauddin Zakariya University Multan, August 24, 2017.
12. Participated in 1<sup>st</sup> National Conference on Emerging Trends in Material Science, Department of Physics Abbotabad University of Science and Technology, October, 5-7, 2017.
13. Oral Presenter in Conference entitled “Strongly Correlated Systems and Nanotechnology” held at Department of Physics Women University Multan, January, 15-17, 2019.
14. Invited Speaker in iiScience International Conference entitled “Light Generation, Sensing and Energy Resources held at Department of Physics Women University Multan, March 2-4, 2020.
15. Invited Speaker in 4<sup>th</sup> International Conference on Materials Science & Nanotechnology MSNANO held at Government College University Faisalabad at March 3-5, 2020.
16. Participant in International E-Conference on Emerging Trends and Innovations in Nanotechnology held at Department of Physics Ripah International University, Lahore, April 9-11,2021.
17. Participant in International Workshop on Nanomaterials of Energy Conversion Emerging Photovoltaic and Optoelectronic Technologies (NEEPO-2021) at NCP, Islamabad September,21-22,2021

18. Oral Presenter in 1<sup>st</sup> International conference on Applied Physics and Engineering at Department of Physics NED Karachi, September,16-17,2021.
19. Speaker in International Symposium Modern Trends in Physics held at Government College University Faisalabad at March 17-18, 2021.
20. Participant in Level 1 Training Program Cohort II organized by ORIC BZU, Multan, May,26-29,2025.

## RESEARCH PUBLICATIONS

### International Publications in impact factor Journals

1. **R.M.Arif Khalil**, Muhammad Iqbal Hussain, Ali Raza, Rabail Fatima, Fayyaz Hussain, Manawwer Alam, Rizwan Wahab, Muhammad Ali, Jamal Abdul Nasir Computational investigation of the phase stability, electronic, optical, phonon spectrum, and elastic behavior of layered perovskites  $\text{Ca}_2\text{XO}_4$  ( $X = \text{Zr}, \text{Hf}$ ) for optoelectronic applications “Journal of Molecular Modeling” (2025) 31:4 <https://doi.org/10.1007/s00894-024-06216-4> (IF:2.1)
2. R.Fatima, **R.M.Arif Khalil**, Muhammad Iqbal Hussain, Fayyaz Hussain, “Computational study of the structural, optoelectronic and thermoelectric properties of scandium-based ternary chalcogenides  $\text{XScSe}_2$  ( $X = \text{Li}, \text{Rb}$ ) for applications in photovoltaic cell” Journal of Computational Electronics 23 (2024) 82. DOI: [10.1007/s10825-023-02110-z](https://doi.org/10.1007/s10825-023-02110-z) (IF:2.2)
3. R.Fatima, **R.M.Arif Khalil**, M.I.Hussain, Fayyaz Hussain “DFT insight into the phase stability, optoelectronic, elastic, vibrational, and thermodynamic properties of metal chalcogenides  $\text{RbKM}$  ( $M = \text{S}, \text{Se}, \text{Te}$ ) for energy harvesting technology” Materials Science in Semiconductor Processing 184 (2024) 1. DOI: [10.1016/j.mssp.2024.108854](https://doi.org/10.1016/j.mssp.2024.108854) (IF:4.2)
4. **R.M. Arif Khalil**, Muhammad Iqbal Hussain, Mushahid Hussain Shah, Tahani. Al Muhimeed, Ghazanfar Nazir, Fayyaz Hussain, Umair Mumtaz, “The exploration of physical properties of 2D MXenes  $\text{M}_3\text{N}_2$  ( $M = \text{Ti}, \text{Hf}, \text{Zr}, \text{Mo}$ ) through the first principles approach: The energy harvesting materials” Computational Materials Science 238 (2024) 112947 DOI: [10.1016/j.commatsci.2024.112947](https://doi.org/10.1016/j.commatsci.2024.112947) (IF :4.2)
5. **R.M. Arif Khalil**, Mushahid Hussain Shah, Muhammad Iqbal Hussain, Nouf H. Alotaibi, Saikh Mohammad, Fayyaz Hussain, Ghulam Meeladi, “Ab-initio study about the structural, optoelectronic, magnetic, and elastic properties of novel combinations of 2D MXenes  $\text{M}_3\text{C}_2$  ( $M = \text{Zr}, \text{Mo}$ ) for energy harvesting applications” Physica B:

6. Ibrar Ali Shah, Muhammad Imran, Fayyaz Hussain, Umbreen Rasheed, Ammar Mohamed Tighezza, **R.M.A. Khalil**, Muhammad Shoaib, Muhammad Fahad Ehsan, "Exploration of lead-free novel double perovskite halides  $\text{Na}_2\text{TlBiX}_6$  ( $X = \text{Cl}, \text{Br}, \text{I}$ ) for flexible memory devices: Using DFT approach" *Materials Chemistry and Physics* (2024) 324 (2024) 129680 DOI: [10.1016/j.matchemphys.2024.129680](https://doi.org/10.1016/j.matchemphys.2024.129680) (IF:4.3)
7. **R.M.A. Khalil**, Muhammad Iqbal Hussain, Shumaila Zafai, Rabail Fatime, Nouf H. Alotaibi, Saikh Mohammad, Fayyaz Hussain, Ayesha Asma, Jamal Abdul Nasir "Comprehensive analysis of the phase stability, optoelectronic, mechanical, thermodynamic, and vibrational properties for prospective optoelectronic applications of novel combinations of chalcogenides  $\text{XScF}_2$  ( $X = \text{Li}, \text{Rb}$ ) by employing density functional theory" *May 2024 Journal of Materials Science* 59(2024)1 DOI:[10.1007/s10853-024-09677-3](https://doi.org/10.1007/s10853-024-09677-3) (IF:3.5).
8. Mushahid Hussain Shah, **R.M.A. Khalil**, Muhammad Usman, Muhammad Iqbal Hussain, Fayyaz Hussain, Muniyah Albaqami, Saikh Mohammad, Jamal Abdul Nasir "First-Principles prediction of the structural stability, optoelectronic, magnetic properties and mechanical response of olivine type  $\text{LiMPO}_4$  ( $M = \text{Ni}, \text{Cu}$ ) phosphate materials for energy storage applications" *Computational and Theoretical Chemistry* 1235(2024):11457 DOI:[10.1016/j.comptc.2024.114579](https://doi.org/10.1016/j.comptc.2024.114579).(IF:3.0)
9. Muhammad Ali, **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Fayyaz Hussain "Exploration of the structural, optoelectronic, magnetic, elastic, vibrational, and thermodynamic properties of molybdenum-based chalcogenides  $\text{A}_2\text{MoSe}_4$  ( $A = \text{Li}, \text{K}$ ) for photovoltaics and spintronics applications: a first-principle study" *Journal of Molecular Modeling* (2023) 29:347 <https://doi.org/10.1007/s00894-023-05751-w>.
10. Muhammad Sajid, Maria Ishaque, Muhammad Imran, Niaz Ahmad Niaz, Fayyaz Hussain, Umbreen Rasheed, R. M. Arif Khalil, Syed Mansoor Ali, Sardar Sikandar Hayat, Muhammad Shoaib "Theoretical occurrence of quantized chemistry of conduction mechanism in layered perovskite for the application of Resistive Random Access Memory devices *International Journal of Quantum Chemistry* (2023)27281 <https://doi.org/10.1002/qua.27281>.
11. Shoaib Muhammad, G. Murtaza, Abida Azam, H. H. Raza, R. M. Arif Khalil, Muhammad Iqbal Hussain, and M. Waqas Iqbal "Tailoring magnesium-based hydrides

as potential and reversible materials for solid-state hydrogen storage: A first-principles study [International Journal of Modern Physics B \(2023\)10:1142.](#)

[https://www.worldscientific.com/doi/10.1142/S0217979224503582.](https://www.worldscientific.com/doi/10.1142/S0217979224503582)

12. Niaz Ahmad Niaz , Abdul Shakoor, Fayyaz Hussain, Syed Mansoor Ali, Umar Mahmood, Atsushi Inoishi<sup>4</sup>, Rana Muhammad Arif Khalil and Duncan H. Gregory" Improved structural, electronic, and electrochemical properties of MoS<sub>2</sub>/graphene oxide composite for Li-ion batteries applications" J Mater Sci: Mater Electron (2023) 34:1942 J Mater Sci: Mater Electron (2023) 34:1942 <https://doi.org/10.1007/s10854-023-11212-0>
13. Rabail Fatima, **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Fayyaz Hussain, Computational study of structural, optoelectronics and thermoelectric properties of scandium-based ternary chalcogenides XScSe<sub>2</sub> (X = Li, Rb) for applications in photovoltaic cell, Journal of Computational Electronics (2023) <https://doi.org/10.1007/s10825-023-02110-z>.
14. **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Bushra Karim , Hind Albalawi, Khalid I. Hussein, Fayyaz Hussain, "DFT-based systematic study on the structural, optoelectronic, thermodynamic, vibrational, and mechanical behavior of Ruddlesden Popper perovskites Sr<sub>2</sub>XO<sub>4</sub> (X = Zr, Hf) for optoelectronic applications" International Journal of Quantum Chemistry(2023)e27216 <https://doi.org/10.1002/qua.27216>
15. Malik Shafqat Hayat, **R.M. Arif Khalil** "Ab-initio exploration of unique and substantial computational properties of double hydrides Cs<sub>2</sub>CaTiH<sub>6</sub>, Cs<sub>2</sub>SrTiH<sub>6</sub>, & Cs<sub>2</sub>BaTiH<sub>6</sub>, for the computational manufacturing of hydrogen fuel cell: A DFT study" Journal of Molecular Graphics and Modelling 125 (2023) 108600 <https://doi.org/10.1016/j.jmgm.2023.108600>
16. Farhana Kousar, Umbreen Rasheed, Muhammad Imran, Fayyaz Hussain, Niaz Ahmad Niaz , Syed Mansoor Ali , Muhammad Ali Shar, **R.M. Arif Khalil**, Muhammad Naeem Ashiq, Sadia Khalid "First principle investigation of metallic ion conduction mechanisms in oxide materials for optical responsive storage devices" PhysicaB:Condensed Matter 665 (2023) 415070 DOI [10.1016/j.physb.2023.415070](https://doi.org/10.1016/j.physb.2023.415070)
17. Bisma Tariq , G. Murtaza , Hassan Ali , Samia Razzaq , **R.M. Arif Khalil** , Muhammad Iqbal Hussain , Khawar Ismail , Ghazanfar Nazir , Nouf

H. Alotaibi “First principles study of the structural, half-metallic ferromagnetism, magnetic, and transport properties of  $KXO_2$  ( $X = Pr, Nd, \text{ and } Pm$ ) hexagonal oxides” Solid State Communications 370 (2023)115229370  
<https://doi.org/10.1016/j.ssc.2023.115229>

18. Saira Kiran, Umair Mumtaz, Aymen Mustafa, Muhammad Imran, Fayyaz Hussain, Umbreen Rasheed, **R. M. A. Khalil**, Ejaz Ahmad Kheraf and Alia Nazira “Correction: An ab initio investigation of the structural, mechanical, electronic, optical, and thermoelectric characteristics of novel double perovskite halides  $Cs_2 CaSnX_6$  ( $X = Cl, Br, I$ ) for optically influenced RRAM devices” Royal Society of chemistry 13(19)(2023)12925-12925 <https://doi.org/10.1039/D3RA00078H>
19. Malik Shafqat Hayat , **R.M. Arif Khalil** “A DFT engineering of double halide type perovskites  $Cs_2SiCl_6, Cs_2GeCl_6, Cs_2SnCl_6$  for optoelectronic applications” Solid State Communications 361 (2023) 115064 <https://doi.org/10.1016/j.ssc.2023.115064>
20. Ejaz Ahmad Khera, Fayyaz Hussain, **Rana Muhammad Arif Khalil** “The Structural, Electronic, and Optical Characteristics of  $Sb_{2-x}M_xO_3$  ( $M = Cu, Ni, Zn; x = 0.25$ ) for Optoelectronic and Allied Applications: First-Principles Study” Physical Status Solidi (b) 260(2023)2200520. <https://doi.org/10.1002/pssb.202200520>
21. Shafqat Hayat, **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Fayyaz Hussain, Anwar Manzoor Rana · “A DFT study of perovskite type halides  $KBeBr_3, RbBeBr_3,$  and  $CsBeBr_3$  in triclinic phase for advanced optoelectronic devices” Solid State Communications 344(2022)114674.<https://doi.org/10.1016/j.ssc.2022.114674>  
(IF:1.840)
22. **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Fayyaz Hussain, Nadia Luqman Anwar Manzoor Rana “DFT based study of the structural, optoelectronic, mechanical and magnetic properties of  $Ti_3AC_2$  ( $A=P, As, Cd$ ) for coating applications” Royal Society of Chemistry Advances **12** (2022) 4395-4407.  
<https://doi.org/10.1039/D1RA07856A>(IF:3.361)
23. R. M. Arif Khalil, Muhammad Iqbal Hussain, Saba Arshad, Fayyaz Hussain, Anwar Manzoor Rana ,Hafiz M.Asif Javed “FIRST-PRINCIPLES SIMULATION: STUDY OF THE STRUCTURAL, ELECTRONIC, MECHANICAL AND OPTICAL PROPERTIES OF DISULFIDE  $XS_2$  ( $X=Ta, Ti$ ) COMPOUNDS FOR

OPTOELECTRONIC APPLICATIONS” *Surface Review and Letters* 29 .06(2022) 2250083. <https://doi.org/10.1142/S0218625X22500834> (IF:1.152)

24. Ejaz Ahmad Khera, Chandreswar Mahata, Muhmmad Imran Niaz Ahmad Niaz Fayyaz Hussain, R. M. Arif Khalil, Umbreen Rasheed and SungjunKim “Improved resistive switching characteristics of a multi-stacked  $\text{HfO}_2/\text{Al}_2\text{O}_3/\text{HfO}_2$  RRAM structure for neuromorphic and synaptic applications: experimental and computational study” *RSC Adv.*, 12 (2022) 11649-11656. <https://doi.org/10.1039/D1RA08103A>
25. Ejaz Ahmad Khera, Ubreen Rasheed, Muhmmad Imran, Hafeez Ullah, Fayyaz Hussain, R. M. Arif Khalil, Farhana Kousar, Muhammad Qasim, An insight into structural, electronic and optical characteristics of  $\text{Mo}_{1-x}\text{M}_x\text{O}_3$  (M = Zr, Y, ZrY) for the formation of conducting filaments in optoelectronic memory devices: A first principles study *OPTIK* 258 (2022)168913. <https://doi.org/10.1016/j.ijleo.2022.168913>.
26. S. Kiran , U. Rasheed , M. Imran , F. Hussainb , N. A. Niazb , E. A. Kherad , R. M. A. Khalilb , A. Nazir “Theoretical investigation of doped  $\text{LiMg}_{1-x}\text{Y}_x\text{N}$  (Y = Ag, Cu, Mn, Zn) for RRAM application” *J.Ovonic Research* 18 (2022)301-315. <https://doi.org/10.15251/JOR.2022.183.301> . (IF:0.892).
27. Syed Awais Rouf, Muhammad Iqbal Hussain, Umair Mumtaz, Hafiz Tariq Masood, Hind Albalawi, Abdul Mannan Majeed, R M Arif Khalil and Q Mahmood “An *ab-initio* study of electronic and optical properties of  $\text{RhXO}_3$  (X = Ga, Ag) perovskites” *Physica Scripta* 97,2 (2022). <http://dx.doi.org/10.1088/1402-4896/ac4b34>.
28. **R. M. Arif Khalil**, Muhammad Iqbal Hussain, A.M.Rana, Fayyaz Hussain, Neelam Inam, H.H.Somaily, Shafqat Hayat First principles study of the structural, optoelectronic and mechanical properties of  $\text{XLaS}_2$  (X=Cu, Zn) for optoelectronic applications 258 (2022)168940 <https://doi.org/10.1016/j.ijleo.2022.168940>.
29. Samia Razzaq, G.Murtza, R.M.Arif Khalil. Nazir Ahmad, Hafiz Hamid “Ab-initio calculation of electronic, mechanical, optical and phonon properties of  $\text{ZrXH}_3$  (X = Co, Ni and Cu): A key towards potential hydrogen storage materials” *Interntional Journal of Modern Physics B* (2022) <http://dx.doi.org/10.1142/S0217979222500904>;
30. Hina Gul, Hafiz Muhammad Asif Javed, Muhammad Awais, Muhammad Yasar Javaid, M. Ijaz Khan, Muhammad Arif, Mohammad Y. Alshahrani, **Rana Muhammad Arif**

**Khalil**, Falak Sher Khan & Ahmed M. “TiO<sub>2</sub> nanoparticles functionalized with marigold for antioxidant role to enhance the skin protection” *Biomass Conversion and Biorefinery* (2022) <https://doi.org/10.1007/s13399-022-02433-0>

31. Amjad Ali, Sajid Munir, Mubushar Majeed, **Arif Khalil**, Muhammad Iqbal Hussain, and Rizwan Raza “Effect of Manganese Catalysts on the Performance of Anodes in Direct Carbon Fuel Cells” *ACS Appl. Energy Mater.* 2022,5,6,6878(2022)6878-6885. <https://doi.org/10.1021/acsaem.2c00450>
32. **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Nyla Saeed, Fayyaz Hussain, Anwar Manzoor Rana, Amjad Ali, H.H. Somoily “Exploration of the structural, optoelectronic and vibrational behavior of Sb<sub>2</sub>S<sub>3</sub> through the first principles approach for phenomenal applications in solar cells” *Optical and Quantum Electronics* **54** 779 (2022).
33. Muhammad Iqbal Hussain and **R.M. Arif Khalil** “Density functional theory studies of the structural, optoelectronic, bond stiffness and lattice dynamical properties of double perovskite oxides M<sub>2</sub>YVO<sub>6</sub> (M= Mg, Sr): Promising candidates for optoelectronic applications” *Materials Science in Semiconductor Processing* 152(28) (2022) 107050.
34. Ayesha Zia G. Murtaza, Khawar Ismail R.M. Arif Khalil Muhammad Iqbal Hussain “Ab-initio calculations of the structural, electronic and optical response of KXCl<sub>3</sub> (X = Be, Ca and Sr) for optoelectronic applications” *Computational Condensed Matter* HYPERLINK "https://www.sciencedirect.com/journal/computational-condensed-matter/vol/33/suppl/C" \_\_\_\_\_ 33, (2022), e00737. <https://doi.org/10.1016/j.cocom.2022.e00737>
35. Umbreen Rasheed, Muhammad Imran, R.M. Arif Khalil. Muhammad Naeem Ashiq Chandreswar Mahata, Fayyaz Hussain “Theoretical exploration of site selective Perovskites for the application of electronic and optoresponsive memory devices” *Physica E* 145 (2023) 115514.
36. Umbreen Rasheed, Muhammad Imran, Abdul Shakoor, Niaz Ahmad Niaz, Fayyaz Hussain, Rana Muhammad Arif Khalil, Mohammad Alkhedher and Sayed M. Eldin “Theoretical Investigation of Origin of Quantized Conduction in 2D Layered Ruddleson–Popper Perovskite Heterostructure for the RRAM Applications” *Energies* **2022**, 15(24), 9410. <https://doi.org/10.3390/en15249410>

37. **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Nyla Saeed, Anwar Manzoor Rana ·  
Fayyaz Hussain “The prediction of structural, electronic, optical and vibrational  
behavior of ThS<sub>2</sub> for nuclear fuel applications: a DFT study” Optical and Quantum  
Electronics (2021) 53:11 <https://doi.org/10.1007/s11082-020-02698-7> (IF:1.842)
38. **R. M. Arif Khalil**, Muhammad Iqbal Hussain Anwar Manzoor Rana, Fayyaz  
Hussain “DFT based first principles study of novel combinations of perovskite-type  
hydrides XGaH<sub>3</sub> (X = Rb, Cs, Fr) for hydrogen storage applications” AIP Advances 11,  
025032(2021) <https://doi.org/10.1063/5.0037790>. (IF:1.456)
39. Umbreen Resheed, Turki Alsuwian, Muhammad Imran, Hassan Algadi, Ejaz Ahmad  
Khera, **R. M. Arif Khalil**, Chandreswar Mahata, Fayyaz Hussain “Density functional  
theory insight into metal ions and vacancies for improved performance in storage  
devices” International Journal of Energy Research 45 (2021)10882  
<https://doi.org/10.1002/er.6572>. (IF:3.741).
40. **R.M. Arif Khalil**, Muhammad Iqbal Hussain, Muhammad Imran, Fayyaz Hussain,  
Nyla Saeed, G. Murtaza, Anwar Manzoor Rana, and Chandreswar Mahta “First-  
Principles Simulation of Structural, Electronic and Optical Properties of Cerium  
Trisulfide (Ce<sub>2</sub>S<sub>3</sub>) Compound” Journal of Electronic Materials 50 (2021) 1637-1641  
<https://doi.org/10.1007/s11664-020-08478-z> . (IF:1.774).
41. **R. M. Arif Khalil**, Muhammad Iqbal Hussain, Ayesha Batool, ,Fayyaz Hussain, Anwar  
Manzoor Rana, Nadia Luqman “Computational study of TbMn<sub>2</sub>O<sub>5</sub> and Tb<sub>2</sub>MnCoO<sub>6</sub>  
to probe the structural, vibrational and optoelectronic properties using PBE + U  
Functional” OPTIK- International Journal of Light and Electron Optics 241 (2021)  
166835. <https://doi.org/10.1016/j.ijleo.2021.166835>. (IF:2.187)
42. Marriam Zahra. Amjad Ali **Arif Khalil** , Saif Ur Rehman, Naveed Mushtaq  
Muhammad Akbar, Rizwan Raza “Studies of electrical and optical properties of  
cadmium-doped zinc oxide for energy conversion devices” Fuel Cells 21 (2021) 164  
<https://doi.org/10.1002/fuce.202000026>. (IF:1.876)
43. Shafqat Hayat, **R. M. Arif Khalil**, Muhammad Iqbal Hussain Anwar Manzoor Rana  
,Fayyaz Hussain, “First-principles investigations of the structural, optoelectronic,  
magnetic and thermodynamic properties of hydride perovskites XCuH<sub>3</sub> (X = Co, Ni,  
Zn) for hydrogen storage applications” OPTIK-International Journal of Light and

Electron Optics 228 (2021)166187. <https://doi.org/10.1016/j.ijleo.2020.166187>  
(IF:2.187)

44. G. Murtaza , Thamraa Alshahrani , R.M. Arif Khalil , Q. Mahmood , Tahani H. Flemban , Hind Althib , A. Laref “Lead Free Double Perovskites Halides  $X_2AgTiCl_6$  ( $X = Rb, Cs$ ) for solar cells and renewable energy applications” Journal of Solid State Chemistry 297 (2021) 121988. <https://doi.org/10.1016/j.jssc.2021.121988> (IF:2.726)
45. Ejaz Ahmad Khera , Hafeez Ullah, Muhammad Imran, Niaz Ahmad Niaz , Fayyaz Hussain , **R.M. Arif Khalil** , Umbreen Resheed , Anwar Manzoor Rana , Muhammad Iqbal Hussain , Chandreswar Mahata , Sungjun Kim “ab initio study of oxygen vacancy effects on structural, electronic and thermoelectric behavior of  $AZr_{1-x}M_xO_3$  ( $A = Ba, Ca, Sr; M = Al, Cu, x = 0.25$ ) for application of memory devices” Journal of Molecular Graphics and Modelling 103 (2021) 107825. <https://doi.org/10.1016/j.jmgm.2020.107825> (IF:2.079)
46. Yu-Ming Chu, Hafiz Muhammad Asif Javed , Muhammad Awais , Muhammad Ijaz Khan, Sana Shafqat, Falak Sher Khan , Muhammad Salman Mustafa, Dawood Ahmed Sami Ullah Khan and **Rana Muhammad Arif Khalil** “Photocatalytic Pretreatment of Commercial Lignin Using  $TiO_2$ -ZnO Nanocomposite-Derived Advanced Oxidation Processes for Methane Production Synergy in Lab Scale Continuous Reactors” Catalysts 11 ( 2021) 54. <https://doi.org/10.3390/catal11010054> (IF:3.520)
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#### **Book Chapter Publications:**

- Muhammad Imran, Fayyaz Hussain, Abdul Rehman, **R. M. Arif Khalil**, Tariq Munir, M.Zeeshan Yaqoob, Sungjun kim (International Book Chapter) “ Simulation Studies for Black Phosphorous: From Theory to Experiment” Engineering Materials Book Series Springer Nature Switzerland (2020) 101-115. <https://doi.org/10.1007/978-3-030-29555-4>.
- Umbreen Rasheed, Fayyaz Hussain, Muhammad Imran, **R.M.Arif Khalil**, Sungjun Kim, “Layered 2D Advanced Materials and Their Allied Applications”, John Wiley HYPERLINK "https://www.bookdepository.com/publishers/John-Wiley-Sons-Inc"& HYPERLINK "https://www.bookdepository.com/publishers/John-Wiley-

Sons-Inc"\_\_Sons\_\_Inc New York United States (2020) 141-158.

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**REVIEWED PUBLICATIONS/LAB MANUAL:**

1. Various Elsevier/Wiley (Publishers) articles have been reviewed till date.
2. Reviewed Lab Manual entitled “Experiments in Analog Electronics” for BS/Master level students of Electronics Lab which has been published by the New Books N Books Multan in 2018.