

Name	Dr. Maria Khalil		
Education Details	Degree	Board/ University	Div./Grads
	PhD- Physics	University of the Punjab, Lahore, Pak	3.95/4.00
	M.Phil.-Physics	MUST- Mirpur AJK	1st Division
	BS -Physics	University of Gujrat (UOG), Pak	1st Division
	F.Sc	AJK BISE-Mirpur	1st Division
	Matric (Science)	AJK BISE-Mirpur	1st Division
Point of Contact	maria.phy@must.edu.pk Maria Khalil, Lecturer, Department of Physics, MUST, Jari Kass Campus, Mirpur, AJK		
Experience:-	11 year		
Honours and Awards	Received a laptop through the Prime Minister's Laptop scheme in BS program.		
Service Activity	Teaching, research, and departmental focal person (Scholarships)		
Brief Statement of Research Interest	Materials science and condensed matter physics		
Publications	<ol style="list-style-type: none"> 1. Khalil, M., Bashir, A., Ullah, F., Ramay, S. M., & Saleem, M. (2025). Tailoring the properties of ZrO₂ through praseodymium doping: a combined DFT and experimental investigation. <i>Materials Science and Engineering: B</i>, 319, 118374. I.F=4.6 2. Alharthi, A. I., Ahmad, P., Khalid, A., Bibi, S., Khalil, M., & Saleem, M. (2025). A comprehensive study on Sr_xCa_{1-x}TiO₃ perovskites using DFT and experimental approach for thermoelectric and optical applications. <i>Inorganic Chemistry Communications</i>, 115080. I.F=5.4 3. Qureshi, M. T., Farooq, U., Al Elaimi, M., Affan, H., Yunus, G., Mohammed, A. M., Khalil, M., & Saleem, M. (2025). Comparative simulation and experimental investigations on Ba_{1-x}Ca_xTiO₃ perovskites for optical and thermoelectric applications. <i>Results in Physics</i>, 108316. I.F=4.6 4. Farooq, U., Qureshi, M. T., Yunus, G., Mohammed, A. M., Ali, A. W. M., Salem, M. S. Khalil, M., & Saleem, M. (2025). Exploring thermoelectric and optical response of Zn_xW_{1-x}O₃ using comparative simulation and experimental techniques. <i>Physica Scripta</i>. I.F=2.6 5. Rouf, H. T., Zeeshan, T., Khalil, M., Ullah, F., Ramay, S. M., & Saleem, M. (2025). DFT and experimental study of Mg substituted strontium oxide for optoelectronic applications. <i>Journal of Physics and Chemistry of Solids</i>, 		

112656. **I.F=4.9**

6. Rouf, H. T., Zeeshan, T., **Khalil, M.**, Ullah, F., Ramay, S. M., & Saleem, M. (2025). DFT and experimental approach: Ca substituted strontium oxide thin films for optoelectronics: HT Rouf et al. *Optical and Quantum Electronics*, 57(6), 352. **I.F=4.0**
7. Farooq, U., Qureshi, M. T., Mohammed, A. M., Al Elaimi, M., Affan, H., Salem, M. S., **Khalil, M.**, & Saleem, M. (2025). Simulation and experimental investigations for influence of Ca doping on electronic, thermoelectric and optical properties of MgO. *Physica B: Condensed Matter*, 701, 416962. **I.F=2.8**
8. Qureshi, M. T., Farooq, U., Yunus, G., Mohammed, A. M., Hussein, A. W., Rehman, W. **Khalil, M.**, & Saleem, M. (2025). DFT and experimental investigations on structural, electronic, thermoelectric, and optical properties of Zn doped PbS. *Applied Physics A*, 131(4), 1-12. **I.F=2.6**
9. Qureshi, M. T., Farooq, U., Al Elaimi, M., Affan, H., Salem, M. S., **Khalil, M.**, ... & Saleem, M. (2025). DFT and experimental investigations on Gd doped CeO₂ for electronic, thermoelectric and optical properties. *Ceramics International*. **I.F=5.6**
10. **Khalil, M.**, Qureshi, M. T., Al Elaimi, M., Aamir, L., Ahmad, M., Saleem, M., & Saleem, M. (2024). Influence of Sr doping on BaTiO₃ properties: A combined DFT and experimental approach. *Results in Physics*, 108041. **I.F=4.6**
11. Ikhlaq, U., Sami, S., **Khalil, M.**, Ullah, F., Ramay, S. M., Ali, S. A., & Saleem, M. (2024). Structural, electronic, and optical properties of Zn-doped V₂O₅ thin films. *Physica Scripta*, 99(9), 095981. **I.F=2.6**
12. Farooq, U., Bibi, S., **Khalil, M.**, Qureshi, M. T., Al Elaimi, M., Aamir, L., ... & Saleem, M. (2024). DFT and experimental investigations on Pr substituted WO₃ for electronic, thermoelectric and optical applications. *Journal of Physics and Chemistry of Solids*, 112192. **I.F=4.9**
13. Sanam, M., Shah, Z. H., Ullah, F., **Khalil, M.**, Ramay, S. M., & Saleem, M. (2024). Structural, electronic, and optical study of Zn: MgO compositions by computational and experimental approach. *Ceramics International*. **I.F= 5.6**
14. **Khalil, M.**, Khalil, U., tu Rouf, H., Ullah, F., Ramay, S. M., & Saleem, M. (2024). Effect of Nd substitution on electronic, thermoelectric, and optical response of WO₃. *Solid State Communications*, 115467. **I.F=2.4**

	<p>15. <u>Khalil, M.</u>, Bashir, A., Ullah, F., Ramay, S. M., & Saleem, M. (2024). Electronic, Optical, and Epsilon Near-Zero Response in Magnetron-Sputtered Tantalum Oxynitride Thin Films. <i>Journal of Electronic Materials</i>, 1-16. I.F=2.5</p> <p>16. <u>Khalil, M.</u>, Bashir, A., Ullah, F., Ramay, S. M., & Saleem, M. (2023). Study of electronic, thermoelectric, and optical response of Zinc Oxynitride thin films. <i>Materials Today Communications</i>, 107332. I.F=4.5</p> <p>17. <u>Khalil, M.</u>, Bashir, A., Alghamdi, E. A., Siddig, A. A., Ramay, S. M., & Saleem, M. (2023). Study of epsilon-near-zero response in Al substituted titanium oxynitride thin films using computational and experimental investigations. <i>Materials Science and Engineering: B</i>, 291, 116369. I.F=4.6</p> <p>18. Iqbal, T., Haq, K. U., Irfan, M., <u>Khalil, M.</u>, Ramay, S. M., Ebdah, M. A., & Saleem, M. (2023). Structural and optical investigations on ZnO-PVDF-NiO advanced polymer composites for modern electronic devices. <i>Materials Research Express</i>, 10(4), 045302. I.F=2.3</p> <p>Book Chapter: Bashir, A., Mehvish, A., & <u>Khalil, M.</u> (2021). Advanced carbon materials for sustainable and emerging applications. <i>21st century advanced carbon materials for engineering applications-A comprehensive handbook</i>.</p>
<p>Selected Professional Presentations</p>	<ul style="list-style-type: none"> ➤ Contributed as Instructor and Trainer for a Hands-on Course on Materials Characterization, held from January 14th -16th, 2025, organized by Central Lab, SBASSE at Lahore University of Management Sciences (LUMS), Lahore. ➤ Principal Instructor and trainer for a hands-on course on Materials Characterization, from October 21st -25th, 2024, organized by Central Lab, SBASSE at Lahore University of Management Sciences (LUMS), Lahore