

بسم الله الرحمن الرحيم

Curriculum Vitae

I. Name: Mohammed Salameh Salem Abu-Jafar

II. Rank: Professor of Physics

Computational Condensed Matter Physics

III. Address:

Department of Physics

An-Najah N. University, P.O. Box 7

Nablus – West Bank

Palestine.

IV. Personal:

A. Date of Birth: July 9, 1960

B. Place of Birth: Jineen-West Bank

C. Marital Status: Married

D. Phone Number: Office: (970)92345113 – Ext. (2475)
Home: (970)92361119

Mobile: (970)599351502

E-mail: mabujafar@najah.edu
mabujafar@yahoo.com

V. Previous Position: Dean of Faculty of Graduate Studies, An-Najah N.

University. P.O. Box 7, Nablus – West Bank, Palestine.

VI. Current Position: Prof. of Physics, Physics Department, An-Najah N.

University, P.O. Box 7, Nablus – West Bank, Palestine.

VII. Degrees and Education:

<u>University</u>	<u>Degree</u>	<u>Date Conferred</u>
An-Najah University-Palestine	B.Sc.	April 1982
Jordan University-Jordan	M.Sc.	Jan. 1985
Southern Illinois Univ.-U.S.A	Ph.D.	Nov. 1991

VIII. Scholarships:

1. Jordan university Scholarship, Jordan, 1982 - 1984.
2. S.I.U Teaching Assistant Scholarship, U.S.A, 1987 - 1991.
3. DAAD Sponsored visit, Bochum University, Germany – Summer 1998.
4. Erasmus Mundus-EPIC scholarship, Postdoc, La Sapienza University, Rome, Italy, Sep. ,10,2014-June,28,2015

IX. Professional Experiences:

Oct. 2018- Present:	F u l l Professor of Physics, An- Najah N. University, Nablus, Palestine.
Aug. 2008-Aug.2014:	Dean of Faculty of Graduate Studies
Sep.2004-Sep.2007:	Chairman, Graduate Studies Department for Natural Science, An- Najah N. University.
Sep.2001- Sep. 2003:	Chairman, Physics Department, An- Najah N. University
Jan. 2002- 2018:	Associate Professor of Physics, An- Najah N. University, Nablus, Palestine.
Jan. 1992-Oct.2001:	Assistant Professor of Physics, An-Najah N. University, Nablus, Palestine.
Jan. 1987-Dec. 1991:	Teaching Assistant, Southern Illinois

University – Carbondale, (U.S.A.)

Jan. 1985-Aug. 1986: Lecturer, An-Najah N. University - Nablus
Palestine.

Aug.1982-Jan.1985: Teaching Assistant, Jordan University-
Amman, Jordan.

X. Administration Experience:

1- Chairman, Department of Physics, An-Najah N. University
(2001 - 2003).

2- Chairman, Department of Graduate Studies for Natural
Sciences, An-Najah N. University (2004 - 2007).

3- Acting Dean of Faculty of Graduate Studies, An-Najah N.
University (Spring semester, 2006/2007).

4- Dean of Faculty of Graduate Studies, An-Najah N. University
(2008 – 2014).

XI. Teaching Experience:

1- Undergraduate Theoretical Courses:

Quantum Mechanics (I & II), Classical Mechanics (I & II), Mathematical Physics (I & II), Solid State Physics, Modern Physics (I & II), Thermodynamics, Electromagnetic Theory, Atomic & Molecular Physics, Statistical Physics, Special Topics, Scientific Research, Computer in Physics, Optics and General Physics (I, II & III).

2- Graduate Courses:

Quantum Mechanics (I & II), Classical Physics, Atomic & Molecular Physics, Mathematical Physics, Nuclear Physics, Solid State Physics and Special Topics.

XII. Master & Ph.D. Thesis Supervision:

1. Sana'a A. Ghanem, "FP-LAPW Calculations of the Structural Phase Transformations of ZnSe & ZnS under High Pressure", 2003.
2. Saja Ibrahim Abdal-Hadi, "The Melting Dynamics of Nanoscale Pd Clusters", (Co-Supervision with Dr. Najeh Jisrawi), 2003.
3. Omer Mahmood Isleem, "XO (X=Be, Zn) Compounds under High Pressure", 2008.

4. Farah Ali Saleh, "Ga_{1-x} Mn_x N Magnetic Semiconductors: First-principles Study", 2008.
5. Raed Tawfeeq Jaradat, "Electronic, Structural and Magnetic properties of Al_{1-x} Mn_x N in Zincblende Structure: First Principle Study", 2009.
6. Haneen Yousef Saeed Shalash, "FP-LAPW Study of Phase Changes in AN (A=Al, In, and B) under High Pressure, 2009.
7. Kamal Falah Mostafa, "FP-LAPW calculations of the electronic properties and structural phase transitions in CoO and CdO", 2009.
8. Hani Ghalib Daraghme, "Electronic and Structural Properties of ScSb and ScP compounds under High Pressure", 2009.
9. Mahmoud Mohammed Eissa, "Structural, Electronic and Magnetic Properties of Ga_{1-x} Fe_x N (x=0, 0.25, 0.75, 1) Alloy in Zincblende Structure: First – Principles Study", 2010.

10. Samia Omer Al-Deek,” The Impact of Computer Simulation to Achieve Immediate and Deferred Eleventh Grade and Their Attitudes towards the Unit Mechanics and Mentor”, 2010.
11. Eman Mohammad Al-Rabi, "Structural, Electronic and Magnetic Properties of $Al_{1-x}V_xP$ Alloys in Zincblende Structure using FP-LAPW Method, 2012.
12. Rowaida Fakhri Dewaikat, "High-Pressure Band Structure and Structural Stability of EuTe and EuO Compounds”, 2012.
13. Iman Jbarah Al-Faqeeh,” The Effect of the Electromagnetic Radiation from High Voltage Transformers on Students Health in Hebron District”, 2014.
14. Mohammed W. Suleiman,” The effect of light intensity on employee’s health in pharmaceutical companies”, 2014.
15. Isra’ Ribhi Abu Hadbah,” Effects of Electromagnetic Radiation from Microwave Ovens on Workers’ Health at Cafeterias in Some Higher Educational Institutions in Palestine”, 2014.
16. Muna Fozan Ahmad Darawshe,” Electric and Magnetic Field Radiation Leakage from Microwave Ovens at Homes in Palestine”, 2014.
17. Reham Issam Thaher,” The effect of electromagnetic radiation from antennas on children in schools in Nablus area”, 2015.
18. Estiklal Basem Fuqha,” Determination of Some Metallic Elements and their Effect on Physical Properties of Edible Olive Oil in Palestine”, 2015.
19. Heba Bsharat,” Critical Behavior of Refractive Index of Binary

- Mixture Cyclohexane-Phenol”, 2015.
20. Maryam Reehan,” Critical Behavior of the Ultrasonic Attenuation for the Binary Mixture of Water and Phenol” 2015.
 21. Jihan Marouf Turkey Abu Snouber,” Analysis of Palestinian Olive Oil of Different Storage Ages by Fluorescence Spectroscopy Technique”, 2016.
 22. Ranan Munier Bani Fadel,” Thermal Expansion Anomaly Near the Critical Consolute of Triethylamine-Water”, 2017.
 23. Raed Tawfeeq Aref Jaradat,” FP-LAPW Study of Structural, Electronic, Elastic and Optical Properties of Alkali Hydrides Compounds XH (X=Li, Na, K, Rb, Cs)”, 2018.
 24. Areej M. Shawahni," Structural, Electronic, Elastic & Optical Properties of SrRhO₃, SrZrO₃ and SrTiO₃ Compounds: FP-LAPW Study", 2018.

25. Doha Naser Abu Baker," Structural, electronic, magnetic & elastic properties of Full-Heusler alloys: normal and inverse Zr_2RhGa , $CoTiSn$ using FP-LAPW method", 2018.
26. Rowaida Mahmoud Esa Sadeq," Modification of the Kawasaki's Analytic Function in Binary Liquid Mixtures", 2019.
27. Sara Jamal Mohammad Yahya," Structural, electronic, magnetic and elastic properties in the Full-Heusler Compounds: Co_2CrAl , Cr_2MnSb using FP-LAPW Method", 2021.
28. Zainab Mualla," Structural, Elastic and Electronic Properties of: KI and RbI compounds", 2021.
29. Khadejah Al-Masri," Structural, electronic, magnetic and elastic properties of the Full-Heusler Compounds: Sc_2TiAl , Sc_2TiSi using FP-LAPW Method", 2022.
30. Omar Rustum Mushref Kabi ," Structural, Electronic, Magnetic and Elastic properties of $CeCrO_3$, $CeGaO_3$ compounds by using: FP-LAPW Study", 2022.
31. Rowaa Jallad," Structural, Electronic, Elastic and Magnetic Properties of: $SmCrO_3$ and $SmMnO_3$ Compounds", 2022.
32. Noorhan Fareed Alshaikh Mohammad, "Investigation on electronic, magnetic, elastic, optical, thermodynamic and thermoelectric properties of $CoCrZ$ ($Z = S, Se, Te$) Half-Heusler compounds using FP-LAPW

method”, 2024.

33. Ruba Zahi Theeb Al-Gharabah, “STRUCTURAL, ELECTRONIC, MAGNETIC, AND ELASTIC PROPERTIES OF THE FULL-HEUSLER COMPOUNDS: Sc_2ZrAl , Sc_2ZrIn USING FP-LAPW METHOD”, 2024.
34. Salma Naser Darweesh Braik, “STRUCTURAL, ELECTRONIC, MAGNETIC, AND ELASTIC PROPERTIES OF THE FULL-HEUSLER COMPOUNDS: Fe_2MnIn , Au_2MnIn USING FP-LAPW METHOD”, 2024.
35. Duaa Ali Hasan, “STRUCTURAL, ELECTRONIC, MAGNETIC, AND ELASTIC PROPERTIES OF THE Full-Heusler COMPOUNDS: Co_2MnSi , Co_2MnGe USING FP-LAPW METHOD”, 2025.
36. Hasan Ali Hasan Masri, “Exploring the Structural, Mechanical, Electronic, Magnetic, Optical and Thermoelectric Properties of New Quaternary Heusler Alloys FeMnScGa , FeMnScAl and FeMnCrGe ”, 2025.

XIII. External Examiner of Post Graduate Student

1. Nahiel Mi Abu Assab,” Theoretical Study of Some Physical Properties of Cuprite”, Al-Quds University, 2001.
2. Mai Ibrahim Khalel, "Effect of the Surface Charge Discretization (Fixed Charge) on Electronic Double Layer”, Al-Quds University, 2011.
3. Azzam Ali Abu Khalil, "Analytical Model Study of Complications of Linear Polyelectrolyte with a Charged Dendrimer of Different Generations”, Al-Quds University, 2011.
4. Naba’ Adnan Zahran,” Complexation of a Linear Polyelectrolyte with Charged Dendrimers: Polyelectrolyte Length Effect”, Al-Quds University, 2015.
5. Walaa’ Mohammed Najeeb Jubeh,” Hypergeometric Function Representation of Transport Coefficients for Drifting Maxwellian and Drifting bi-Maxwellian Plasmas”, Al-Quds University, 2017.
6. Isra Mazin Zedan,”Analytical study of position dependent mass harmonic oscillator “,”Palestine Technical University-Khadoorie(PTUK), 2023.
7. Rawan Mahmood Mustafa Ghanim,” First Principles Calculation of structural, electronic, elastic, optical and thermoelectric properties of the Half-Heusler compound **ZrPdSn** using FP-LAPW”, Master Thesis, Palestine Technical University-Khadoorie (PTUK), 2024.
8. Arwa Nazeh Tawfeeq Abu Ghannam,” Magnetic and Thermal Properties of Graphene Magnetic Quantum Dot”, PhD Thesis, Arab American University, 2024.
9. Shahd Hazem Ratib Khashan,” Comprehensive analysis: Exploring quaternary Heusler alloys CoMnVTe through first-principles calculation”, Palestine Technical University-Khadoorie(PTUK), Master Thesis, 2025

XIV. Internal Examiner of Post Graduate Students:

1. Naim "Ahmed Rasheed" Malak, "Effect of a uniform Applied Magnetic Field and Temperature on the Magnetic Properties of the Dipolar Anti-ferromagnetic planar systemic Parametric Study", 2008.
2. Baseemeh Daas Zpeedeh, "First Principle Electronic Structure Calculations of Ternary alloys. $\text{BN}_x \text{P}_{1-x}$, $\text{Ga}_x \text{B}_{1-x} \text{N}$ and $\text{B}_x \text{In}_{1-x} \text{N}$ in Zincblende Structure", 2008.
3. Thaer "Mohammed Said" Abu-Labdeh", Influences of a uniform External Magnetic Field on the Magnetic properties of the Dipolar Anti-ferromagnetic Heisenberg System", 2009.
4. Muzaian Abdulhameed Shaqqur, "Confined hydrogen atom in a spherical cavity in N dimensions", 2009.

5. Tajweed Hashim Nierate, "Temperature and Storage Age Dependence of Olive Viscosity in Different Locations in Palestine", 2012.
6. Isra Sulyman Faies Maraaba," Studying the Retention of Multivalent Pollutants in Bentonite", 2014.
7. Saja Mohammad Yousef Abdo,"Intermolecular Force Range and Noncritical Shear Viscosity of the Critical Binary Mixture of Benzene-Coconut Oil", 2014.
8. Yusur Hisham Kittany," Debye Momentum Cutoff of the Critical Binary Mixture of Carbon Tetrachloride and Coconut Oil", 2014.
9. Diya Aldeen Adnan Qasem," Modification of the Fixman's Analytic Function in Binary Liquid Mixtures", 2014.
10. Asmaa Abd Ulkareem Shehade,"Radiation Environment in Selected Healthcare Centers in Palestine", 2016.
11. Tasneem Basim Abdelkareem Abdallah,"Performance Study of Inner Tracker (ITK) in ATLAS at the Large Hadron Collider(LHC at CERN)", 2018.
12. Loay Ali Manasra, " Hexavalent Ions Sorption on Bentonite Clay", 2018.
13. Hend Saleem Shahed, " Flux Simulation and Studies of the First X-Ray Beam of the ThomX Project", 2018.
14. Amal Jawdat Nayef Darawsheh, " Effect of Applied Fields on the Magnetic Properties of Donor Impurity Confined in Parabolic GaAs Quantum Dot", 2018.

15. Theraa Tork, " Tracking Performance in very dense environment for ATLAS Inner Tracker (ITK) at Large Hadron Collider at the European Organization for Nuclear Research (CERN)", 2019.
16. Asma Mazooz, "Rashba Effect on the Magnetic properties of a Two-Dimensional GaAs Quantum Ring with Impurities in an Applied Magnetic Field", 2020.
17. Jeelan Sayyed, " Carbon Nanotube-Composite Material for Dipole Antenna at Terahertz Range, Analysis, Properties, Efficiency and Performance", 2021.
18. Salsabeel Khalel Saleh, " Electric Field Effect in Monolayer of Graphene", 2022.
19. Ayham Anwar Ahmad Shaer "MAGNETIC AND ELECTRONIC PROPERTIES OF InAs ANISOTROPIC DOPED QUANTUM DOT WITH SPIN-ORBIT COUPLING: COMPUTATIONAL STUDY", PhD Thesis, 2023.
20. Hosnia Salahat, "WAFER PROBING MEASUREMENTS OF ITkPix-V1 FOR ITk PIXEL ATLAS UPGRADE", 2024.
21. Mahmoud Majed Ali, " MAGNETOCALORIC EFFECT AND ELECTRONIC PROPERTIES OF DOPED **InSb** -DOUBLE QUANTUM WIRE IN THE PRESENCE OF EM FIELDS AND SPIN-ORBIT TERMS",

XV. Non-Curricular Activities:

- 1- Education activities.
- 2- Swimming.
- 3- Tennis.

XIII. Other Skills:

1. COMPUTER & Software SKILLS

- A) FORTRAN Programming
- B) FP-LMTO Technique
- C) FP-LAPW Technique
- D) Mathematica
- E) Maple

2. VARIATIONAL METHODS

XVI. Current Research Interests:

I - Computational Condensed Matter Physics.

In our research we use the program package WIEN2K which allows us to perform electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential

(linearized) augmented plane-wave (L)APW) + local orbitals (lo) method, one among the most accurate schemes for band structure calculations. In DFT the local (spin) density approximation (LDA) or the improved version of the generalized gradient approximation (GGA) can be used. WIEN2K is an all-electron scheme including relativistic effects and has many features.

Additionally, we use the PWscf (Plane-Wave Self-Consistent Field) which is a set of programs for electronic structure calculations within Density-Functional Theory and Density-Functional Perturbation Theory, using a Plane-Wave basis set and pseudopotentials.

II- Multiperturbation Theory and Its Applications to Polyatomic

Molecules.

Recently computational physics became an important branch of physics because it complements experimental and theoretical physics. Using this relatively new part of physics, one carries out computer experiments to study some physical phenomena, calculate numerically a physical quantity or predict a theoretical model from available experimental data.

The application of high order perturbation theory to the calculation of atomic and molecular properties has several advantages over conventional approaches generally applied to these systems. Molecular surfaces for polyatomic molecules are difficult to compute with any degree of accuracy and very expensive in terms of computing resources. Perturbation theory provides important theoretical and computational simplifications to this problem

while continuing to provide comparable accuracy with a relatively small expenditure of computational resources.

XVII. Committee Membership:

Committees:

University Level

- 1- University Council.
- 2- Many other committees such as student Regulation, Student Union Council Election, Investigation Committees.
- 3- An-Najah N. University prize Establishing Committee (2006/2007).

- 4- An-Najah N. University prize Committee, Chairman (2011/2012).
- 5- Higher Academic Counseling and Supervising Committee (2008-2014).
- 6- Health Insurance Committee (For more than 8 years).

Science College Level

- 1- Board of College of Science.
- 2- Registration & Supervision Committee.
- 3- Library Committee / Coordinator.

Department Level

- 1- Graduate Studies Committee / Coordinator.
- 2- Graduate Student Admission.
- 3- Registration.
- 4- Library Committee / Coordinator.
- 5- Promotion Committee
- 6- Recruiting Committee

XVIII. Professional Activities:

1. Physics graduate committee member, physics department, An-Najah National University, Nablus, West Bank, Palestine, (1996- present).
2. Physics library committee, physics department, An-Najah National University, Nablus, West Bank, Palestine.
3. Coordinator of the computer physics lab for the undergraduate Students.
4. Coordinator of the computational condensed matter physics lab for graduate students.
5. Member of organization committee for physics conference, An-Najah National University, Nablus, West Bank, Palestine, 2000

6. Member of Dean's Council, An-Najah National University, Nablus, West Bank, Palestine, (2008-2014).
7. Member of University Council, An-Najah National University, Nablus, West Bank, Palestine, (2001-2014).
8. Member of organization committee for the second physics conference, An-Najah National University, Nablus, West Bank, Palestine, 2007.
9. Coordinator of the Conference in exploring the future of graduate studies in Palestine, 2009.
10. Coordinator of the International Graduate Conference on Science, Humanities and Engineering, (IGCSHE2011), 2011.
11. Member of organization Committee for Difference and Pluralism from an Islamic Perspective Conference, An-Najah National University, Nablus, West Bank, Palestine, 2012.
12. Member of the guidance and direction supreme (2008-2014).
13. Member of the scientific research committee of the natural science journal, An-Najah N. University(2023-2024)

XIX. Summer Schools, Workshops & Conferences:

- 1 - Twelfth International Conference on Atomic Physics-Ann Arbor-U.S.A., 1990.
- 2 - The First Palestinian Chemical Conference, Nablus-West Bank, Palestine, 1992.
- 3 - Second Symposium on Computational Condensed Matter Physics, Yarmouk University, Irbid-Jordan, 1995.
- 4 - First Workshop on the Applications of Computer for Physics Teaching, Yarmouk University, Irbid, Jordan, 1996.
- 5 - Research Workshop on Condensed Matter Physics, (Electronic Structure, Semiconductor Physics), ICTP, Trieste-Italy, 1996.
- 6 - Workshop on “Modernizing Basic and Engineering Sciences University Education Through Computational and Networking Technologies”, Jordan University for Science and Technology, Irbid-Jordan, 1997.
- 7 - Colleges on Advanced Computational Physics, ICTP-Trieste-Italy, 1997.
- 8 - Third Symposium on Computational Condensed Matter Physics, Yarmouk University, Irbid-Jordan, 1997.
- 9 - Multimedia Workshop, Birzeit University, Palestine, 1998.
- 10- An International Workshop on LAPW, ICTP, Trieste-Italy, 1998.
- 11- Scholarship from DAAD Ruhr-University, Bochum-Germany, 1998.
- 12- Fourth Symposium on Condensed Matter Physics (Advances in High

- Tc-Superconductivity), Yarmouk University, Irbid-Jordan, 1999.
- 13- The Palestinian Physics Conference “Condensed Matter and Applications”, Member of The Organising Committee, An-Najah N. Univ., Nablus, Palestine, 2000.
 - 14- Spring College on Electronic Structure Approaches to the Physics of Materials, ICTP-Trieste-Italy, 2000.
 - 15- Second Physics Conference -2007, Member of the Organising Committee, An-Najah N. University, Nablus, Palestine, 2007.
 - 16- Exploring the Future of Graduate Studies in Palestine, Member of the organizing committee, Faculty of Graduate Studies, An-Najah N. University, Nablus, Palestine, 2009.
 - 17- First Yarmouk School for Computational Condensed Matter and Nano Technology, Yarmouk University, Irbid – Jordan, 2010
 - 18- International Graduate Conference on Science, Humanities and Engineering 2011(IGCSHE2011), Coordinator, Faculty of Graduate Studies, An-Najah N. University, Nablus, Palestine, 2011.

- 19- The Right to Difference and Pluralism from an Islamic Perspective and the Role of Universities in the Development of this Right”, Member of the organizing committee, An-Najah N. University, Palestine, 2012 .

- 20- Symposium on Mont-Carlo Simulations (MC),
 “Application to Nanomagnetic Particles Systems”, Coordinator, An-Najah N. University, Palestine, 2012 .

- 21- Towards Oxide-Base Electronics: science, sample growth and applications of transition metal oxides, Sapienza University, Rome, Italy, September 22-23, 2014

- 22- Second Conference on Superconductivity and Functional Oxides(SuperFOx) ,La Sapienza University, Rome, Italy, September 24- 26, 2014.

- 23- Second Palestinian International Conference on Material Science and Nanotechnology (PICNM2016), An-Najah N. University, Nablus, Palestine, March 23-24, 2016.

- 24- Eighth International Petra School of Physics ” Physics of Low-Dimensional Systems: Theory and Applications”, University of Jordan, Amman, Jordan, April 11-14, 2016.

25. Fifth Palestinian Conference on Modern Trends in Mathematics and Physics, Arab American University, Jenin, Palestine, July 31-August 2, 2016.

26. The Second Palestinian International Graduate Conference on Natural, Medical and Health Sciences & Humanities (SPIGCNMHSH 2017), An-Najah N. University, Nablus, Palestine, April 20, 2017.

27. WISHEPP-II , 2nd Winter School in HEP, An-Najah N. University, Nablus, Palestine, November 12-17, 2017.
28. 9th Scientific Exhibition, Faculty of Science, An-Najah N. University, Nablus, Palestine, April 17-19, 2018.
29. Sixth Palestine Conference on Modern Trends in Mathematics and Physics, Palestine Technical Univesrity- Kadoorie, Tulkarm, Palestine, Aug 5-8, 2018.
30. "AEM 2018' Advanced Energy Materials, University of Surry, England, 10-12 September 2018.
31. The Third Winter School of High Energy Physics in Palestine (WISHEPP III), An-Najah N. University, Palestine, November 10-16, 2018.
32. Program Meeting for Mathematics and Physics, Palestine Academy for

Science & Technology, Ramallah, Palestine, Dec 22, 2018

33. Simulation-based Sciences and Engineering", Palestine Academy for Science & Technology, Ramallah, Palestine, 7-9 March, 2019.

34. 6th Edition of Advanced Chemistry World Congress, March 27-28,| London, UK, 2025

XX. List of Publications

- 1) N. Saleh, A. Hallak, **M. Abujafar**,” Estimation of Neutron Skyshine and Safety Level from Jordan Van De Graaf Accelerator”, **Applied physics Communications (1986).**
- 2) D. H. Galvan, **M. Abu-Jafar** and F.C. Sanders, “Polyatomic Molecules Via z-dependent, Perturbation Theory-Ground state of H_3^+ ”, **Bull.Am. Phys. Soc. 34 (1989) 1382.**
- 3) **M. Abu-Jafar**, F.C. Sanders, and D.H. Galvan, “Potential Energy
+
Surface for H_3 via z-dependent Perturbation Theory – A Third-order study”, **Twelfth International Conference on Atomic Physics, Ann Arbor (1990).**
- 4) **M. Abu-Jafar** and F.C. Sanders, “A Fourth-order Multiperturbation
+

study of H_3 ", **Bull. Am. Phys. Soc.** **36**, 1243 (1991).

- 5) D. M. Galvan, **M. Abu-Jafar** and F.C. Sanders, "Multiperturbation Approach to Potential Energy Surfaces for Polyatomic Molecules" **J. chem. Phys.**, **Vol. 102**, No. 12 (1995).
- 6) **M. Abu-Jafar**, et al "A Fifth-order Multiperturbation Derivation of Polyatomic Molecules", **An-Najah University Journal For Research (Natural Science)**, **Vol. IV**, No. 10, Sep. (1996).
- 7) S. Musameh, I. Abdulraziq and **M. Abu-Jafar**, "Shielding Effectiveness of Carbon Fiber-Epoxy Composite at Microwave Frequencies", **Bethlehem University Journal**, **Vol. 15** (1996).
- 8) I. Abdulraziq, S. Musameh and **M. Abu-Jafar**, "Shear Viscosity Anomaly Near the Critical Binary System of Nitrobenzene-n- heptane", **Bethlehem University Journal**, **Vol. 16** (1996).
- 9) A. Qteish, **M. Abu-Jafar** and A. Nazzal, "The Instability of the Cinnabar Phase in ZnS Under High Pressure", **J. Phys.: Condens. Matter**, **Vol. 10**, U.K. (1998).
- 10) **M. Abu-Jafar**, "Calculation of Ground state Energy for Linear

++

HeH_2 Through Fifth Order (United Atom Treatment), **An-Najah Univ. J. Res.**, **Vol. 12**, Palestine (1998).

- 11) **M. Abu-Jafar**, A.I. Al-Sharif and A. Qteish, “FP-LAPW and Pseudopotential Calculations of the Structural Phase Transformations of GaN Under High-Pressure”, **Solid State Communications**, Vol. **116** (2000).
- 12) A. I. Al-Sharif, **M. Abu-Jafar** and A. Qteish, “Structural and Electronic Structure Properties of FeSi: The Driving Force Behind The Stability of The B20 Phase”, **J. Phys.: Condens. Matter**, Vol. **13**, U.K. (2001).
- 13) I. Abdelraziq, Z. Majjad, **M. Abu-Jafar**, B. Manasrah, “Special functions, **Deanship of Scientific Research**, An-Najah N. University (2004).
- 14) **M. S. Abu-Jafar**, A. M. Abu-labdeh , M. El-Hasan " The energy band gap of ScN in the rocksalt phase obtained with LDA/GGA +USIC approximations in FP-LAPW method " , **Computational materials science** , Vol. **50** (2010) .
- 15) M.W.Suleiman, **M. AbuJafar**, I. R. Abdelraziq, “The effect of light intensity on employee’s health in pharmaceutical companies”, **Environmental Science**, Vol. **10** ,issue **2** (2015).
- 16) Reham IssamThaher, **Mohammed AbuJafar**, Issam Rashid Abdelraziq”The effect of electromagnetic radiation from antennas on children in schools in Nablus area”, **Environmental Science**, Vol. **10**, issue **3** (2015).

- 17) Iman Al-Faqeeh, **Moahmmed Abu-Jafar**, Issam Rashid Abdelraziq”The effect of the electromagnetic radiation from high voltage transformers on students’ health in Hebron district”,
International Journal of Geology, Agriculture and Environmental Sciences, Vol. 3, issue 1(2015).
- 18) R. Zine El-Kelma, L. Beldi, F. El Haj Hassan, G. Murtaza, R. Khenata, **M. S. Abu-Jafar**, S. Bin Omran and B. Bouhafs” Magnetic ordering and electronic structure of the ternary iron arsenide BaFe_2As_2 ”,
International Journal of Modern Physics B, Vol. 29, No. 23 (2015).
- 19) M. El Amine Monir, R. Khenata, H. Baltache , G. Murtaza, **M. S. Abu-Jafar**, A. Bouhemadou, S. Bin Omran, D. Rached,”Study of structural, electronic and magnetic properties of CoFeIn and Co_2FeIn Heusler alloys” , **Journal of Magnetism and Magnetic Materials, Vol. 394 (2015).**
- 20) Nada T. Mahmoud_, Ahmad A. Mousa, Hassan K. Juwhari, Jamil M. Khalifeh and **Mohammed S. Abu-Jafar**,” Optical dispersion functions of $\text{Co}_{2-x}\text{Eu}_x\text{VSn}$ using ab-initio calculations”, **International Journal of Modern Physics B, Vol. 29, No. 28 (2015).**

- 21) M. Khalfa, H. Khachai, F. Chiker, N. Baki, K. Bougherara, A. Yakoubi, G. Murtaza, M. Harmel, **M. S. Abu-Jafar**, S. Bin Omran and R. Khenata, “Mechanical, electronic and thermodynamic properties of full Heusler compounds Fe_2VX ($\text{X} = \text{Al, Ga}$)”, **International Journal of Modern Physics B**, Vol. 29 (2015).

- 22) E. Fuqha, **M. Abu-Jafar** and I. R. Abderaziq, “Determination of Some Metallic Elements and their Effect on Physical Properties of Edible Olive Oil in Palestine”, **Material Science & Engineering**, Vol. 5, No. 1 (2015).

- 23) Heba Bsharat, **Mohammed Abu-Jafar** and, Issam Abdelraziq,” Critical behavior of refractive index of binary mixture cyclohexane-phenol”, **Physical Chemistry**, Vol. 10, No. 2 (2015).

- 24) M. Jamal, **M. S. Abu-Jafar** and A. H. Reshak, “Revealing the structural, elastic and thermodynamic properties of $\text{CdSe}_x\text{Te}_{1-x}$ ($x=0, 0.25, 0.5, 0.75, 1$)”, **Journal of Alloys and Compounds**, Vol. 667 (2016).

- 25) Samah Al-Qaisi, **M. S. Abu-Jafar**, G. K. Gopir and R. Khenata, ” Electronic, structural and magnetic properties of TbO under pressure: FP-LAPW study”, **Phase Transitions: A Multinational Journal**, Vol. 89, No. 12 (2016).

- 26) A. H. Reshak, **M. S. Abu-Jafar**, and Y. Al-Douri, “Two symmetric n-type interfaces $\text{SrTiO}_3/\text{LaAlO}_3$ in perovskite: Electronic properties from density functional theory”, **Journal of Applied Physics**, Vol.

119, 245303 (2016).

- 27) Raed Jaradat, **Mohammed Abu-Jafar**, Issam Abdelrazik, Rabah Khenata ,Dinesh Varshney, Saad Bin Omran and Samah Al-Qaisi, “High-pressure structural phase transition and electronic properties of the alkali hydrides compounds XH (X = Li, Na)”,**Phase Transitions: A Multinational Journal, Vol. 90, No. 9 (2017).**
- 28) Diana Dahlih , **M. Abu-Jafar**, R. Khenata, Ahmad Mousa , Raed Jaradat, Samah Al-Qaisi , S. Bin Omran,” Structural stabilities and band structure characteristics of platinum nitride (PtN) via first-principles calculations ”, **Chinese Journal of Physics, Vol. 55 (2017).**
- 29) Samah Al-Qaisi, **M.S. Abu-Jafar**, G.K. Gopir, R. Ahmed, S. Bin Omran, Raed Jaradat, Diana Dahlih, R. Khenata,” Structural, elastic, mechanical and thermodynamic properties of Terbium oxide: First-principles investigations”, **Results in Physics, Vol. 7 (2017).**

- 30) M. Jamal , **M.S. Abu-Jafar**, Diana Dahliah ,” Disclosing the structural, phase transition, elastic and thermodynamic properties of $\text{CdSe}_{1-x}\text{Te}_x$ ($x = 0.0, 0.25, 0.5, 0.75, 1.0$) using LDA exchange correlation “, **Results in Physics, Vol. 7 (2017)**.

- 31) Maryam Reehan, **Mohammed Abu-Jafar** and Issam Ashqer,” Critical Behavior of the Ultrasonic Attenuation for the Binary Mixture of Water and Phenol” **Acta Acustica united with Acustica, Vol. 103 (2017)**.

- 32) Diana Dahliah, **M. S. Abu-Jafar**, Ahmad A. Mousa, R. Khenata, S. Bin Omran & Raed Jaradat,” Theoretical investigation of the structural stabilities, elastic properties and band structure characteristics of platinum carbide”, **Phase Transitions: A Multinational Journal, VOL. 91, NO. 3 (2018)**.

- 33) A. Mousa, **M. Abu-Jafar**, D. Dahliah, R. Shaltaf, and J. Khalifeh,” Investigation of the perovskite KSrX_3 ($X = \text{Cl} \ \& \ \text{F}$) compounds, examining the optical, elastic, electronic and structural properties: FP-LAPW study”, Journal of Electronic Materials, Journal of ELECTRONIC MATERIALS, **Vol. 47, No. 1 (2018)**.

- 34) Raed Jaradat, **Mohammed S. Abu-Jafar**, Issam Abdelraziq, Diana Dahliah, Rabah Khenata,” Elastic and thermodynamic properties of alkali hydrides XH ($X=\text{K}, \text{Rb}$ and Cs), **Chinese Journal of Physics, Vol. 56 (2018)**.

- 35) Raed Jaradat, **Mohammed Abu-Jafar**, Issam Abdelraziq, Saad

Bin Omran, Diana Dahliah, Rabah Khenata,” High-pressure structural phase transitions and electronic properties of the alkali hydride compounds XH (X=K, Rb and Cs), **Materials Chemistry and Physics, Vol. 208 (2018).**

- 36) Raed Jaradat, **Mohammed Abu-Jafar**, Issam Abdelrazik, Ahmad

Mousa, Tarik Ouahrani, and Rabah Khenata,” Insight into the structural, electronic, elastic and optical properties of the alkali hydride compounds, XH (X = Rb and Cs)”, **AIP ADVANCES, Vol. 8 (2018).**

- 37) R. Boulechfar, Y. Khenioui, S. Drablia, H. Meradji, **M. Abu-Jafar**, S.

Bin Omran, R. Khenata, S. Ghemid,” Theoretical simulations of the structural stabilities, elastic, thermodynamic and electronic properties of Pt_3Sc and Pt_3Y compounds”, **Solid State Communications, Vol. 273 (2018).**

- 38) Rowaida M. Sadeq, Issam Abdelraziq, **Mohammed Abu-Jafar**, "Modification of the Fixmen's, Kawasaki's, Hornowski's, Mistura's, and Chapan's analytic function in binary liquid mixtures", **Results in Physics, Volume 11 (2018)**.
- 39) Rowaida M. Sadeq, Issam Abdelraziq, **Mohammed S. Abu-Jafar** and Oksana Bilous, " The behavior of sound absorption coefficient for binary mixture nitroethane-isooctane above critical temperature and concentration", **AIP Advances 8 (2018)**.
- 40) Areej M. Shawahni , **Mohammed S. Abu-Jafar** , Raed T. Jaradat, Tarik Ouahrani , Rabah Khenata , Ahmad A. Mousa and Khaled F. Ilaiwi, "Structural, Elastic, Electronic and Optical Properties of SrTMO₃ (TM = Rh, Zr) Compounds: Insights from FP-LAPW Study", **Materials 11 (2018)**.
- 41) Jehan A Snouber, Issam Abdelraziq, **Mohammed Abu-Jafar**, Ahed Zyoud, Hikmat Hilal and Antonella Pasqualone, " Physical and chemical behaviour of NabaliMohassan single-cultivar olive oil duringprolonged storage", **J Sci Food Agric 99 (2019)**.
- 42) Ahmad A. Mousa, Raed Jaradat, Said M. Azar, **Mohammed Abu-Jafar**, Emad K. Jaradat, J. M. Khalifeh and K. F. Ilaiwi, " First principle Investigation of the Structural, electronic and elastic properties of the Laves Phase Compounds SrX₂ (X = Pd and Pt)", **Chinese Journal of Physics 59 (2019)**.

- 43) Doha N. Abu Baker, **Mohammed S. Abu-Jafar**, Ahmad A. Mousa, Raed T. Jaradat, Khaled F. Ilaiwi, R. Khenata, " Structural, magnetic, electronic and elastic properties of half-metallic ferromagnetism full-Heusler alloys: Normal-Co₂TiSn and inverse- Zr₂RhGa using FP-LAPW method", **Materials Chemistry and Physics 240 (2020).**
- 44) M. Boukhtouta, Y. Megdoud, S. Benlamari, H. Meradji, Z. Chouahda, R. Ahmed, S. Ghemid, **Mohammed Abu-Jafar**, S. Syrotyuk, D. P. Rai, S. Bin Omran & R. Khenata , " Predictions on structural, electronic, optical and thermal properties of lithium niobate via first-principle computations", **PHILOSOPHICAL MAGAZINE 100, PART B: CONDENSED MATTER PHYSICS (2020).**
- 45) Ahmad A. Mousa, Samah Al-Qaisi, **Mohammed Abu-Jafar**, Said Al Azar, Raed Jaradat, Jamil M. Khalifeh, Tarik Ouahrani, Rabah Khenata, " Ab initio studies of the structural, elastic, electronic and optical properties of the Ni₃In intermetallic compound", **Materials Chemistry and Physics 249 (2020).**

- 46) Ahmad A. Mousa, Raed Jaradat, **Mohammed Abu-Jafar**, Nada T. Mahmoud, Samah Al-Qaisi, Jamil M. Khalifeh, H. Abusaimh, "Theoretical investigation of the structural, electronic, and elastic properties of TM_3In ($TM = Pd$ and Pt) intermetallic compounds", **AIP Advances** **10** (2020).
- 47) **Mohammed Abu-Jafar**, Rowan Dayton-Oxland, Raed Jaradat, Ahmad A. Mousa & Rabah Khenata, "Structural, electronic, mechanical and elastic properties of Scandium Chalcogenides by firstprinciples calculations", **Phase Transitions: A Multinational Journal**, **VOL. 93**, **NO. 8** (2020)773–783.
- 48) **Mohammed S. Abu-Jafar**, Raed T. Jaradat, A. Abu-Labdeh, R. Khenata, Ahmad A. Mousa "Ab initio studies of structural, electronic and magnetic properties of $Al_{1-x}Mn_xN$ in zinc blende structure", **Computational Condensed Matter** **26** (2021).
- 49) **Mohammed S. Abu-Jafar**, Vincent Leonhardi, Raed Jaradat, Ahmad A. Mousa, Samah Al-Qaisi, Nada T. Mahmoud, Ahmed Bassalat, R. Khenata, A. Bouhemadou "Structural, electronic, mechanical, and dynamical properties of scandium carbide", **Results in Physics** **21** (2021).
- 50) Hazem Abu-Farsakh, **Mohammed Abu-Jafar**, Abdallah Qteish, " Modified Becke-Johnson calculations using norm-conserving pseudopotential plane-wave approach: Systematic analysis", **Materials**

Today Communications, 26 (2021).

<https://doi.org/10.1016/j.mtcomm.2020.101748>

- 51) Ahmad A. Mousa, Tarik Ouahrani, Said M. Azar, **Mohammed S. Abu-Jafar**, Rabah Khenata, Mahmoud Farout,” Stability, elastic and electronic properties of the CsSrI₃ halid perovskite”, **Computational Condensed Matter**, **32 (2022)**.
- 52) Ahmad A. Mousa, Said M. Al Azar, Saber Sâad Essaoud, Khadidja Berarma, Aymen Awad, Nada T. Mahmoud, Emad K. Jaradat, and **Mohammed S. Abu-Jafar**,” Structural, Elastic, Electronic, Magnetic, and Thermoelectric Characteristics of MgEu₂X₄ (X $\frac{1}{4}$ S, Se) Spinel Compounds: Ab-Initio Calculations”, **Phys. Status Solidi B**, **259 (2022)**.
- 53) Amjad W Alsmadi, Nada T Mahmoud, Ahmad A Mousa, **Mohammed S Abu-Jafar** and Hesham Abusaimh “Theoretical prediction of doping iron ions effect on the optoelectronic and magnetic cobalt-based perovskite (Co_{1-x}Fe_xScO₃)”, **Materials Research Express**, **9 (2022)**.
- 54) Sara J. Yahya, **Mohammed S. Abu-Jafar**, Said Al Azar, Ahmad A. Mousa, Rabah Khenata, Doha Abu-Baker and Mahmoud Farout, “The Structural, Electronic, Magnetic and Elastic Properties of Full-Heusler Co₂CrAl and Cr₂MnSb: An Ab Initio Study”, **Crystals**, **12 (2022)**.
- 55) Khadejah M. Al-Masri, **Mohammed S. Abu-Jafar**, Mahmoud Farout, Diana Dahliah, Ahmad A. Mousa, Said M. Azar and Rabah Khenata,” Structural, Elastic, Electronic, and Magnetic Properties of Full-Heusler Alloys Sc₂TiAl and Sc₂TiSi Using the FP-LAPW Method”, **Magnetochemistry**, **9 (2023)**.
- 56) **Mohammed S. Abu-Jafar**, Raed Jaradat, Mahmoud Farout, Areej Shawahneh, Ahmad A. Mousa, Khalid Ilaiwi, Rabah Khenata and Said M. Azar,” Insight into the structural, electronic, optical, and elastic properties of niobium carbide, “**PHASE TRANSITIONS**”, **96 (2023)**.

- 57) Raed T. Jaradat, **Mohammed S. Abu-Jafar**, Mahmoud Farout, Said M. Azar, Rabah Khenata and Ahmad A. Mousa,” Structural, electronic, magnetic, and optical investigations of sodium chalcogenides: First-principles calculations”, **AIP Advances**, **13**(2023).
- 58) Zainab Mualla, **Mohammed S. Abu-Jafar**, Ahmed Bassalat, Hadil Abualrob, Ahmad A. Mousa, Mumtaz Manzoor, R. Sharma, R. Khenata and Mahmoud Farout,” Structural, electronic, and elastic properties of RbI using the FP-LAPW method”, **Modern Physics Letters B**, (2023),
DOI:10.1142/S0217984923501452
- 59) S.N. Behilil, M. Harmel, N. Baki, Y.A. Khachai, R. Ahmed, M. Faizan, N. Badi, **Mohammed S. Abu-Jafar**, R. Khenata,” First-principles prediction of optoelectronic and thermoelectric properties of novel materials A_2PdCl_6 for Photovoltaic Applications”, **Computational Condensed Matter**, (2024).
- 60) L. Boumia, F. Semari, M. Mokhtari, F. Dahmane, **Mohammed S. Abu-Jafar**, A. Boumaza, Muhammad Waqas Iqbal, H. Meradji, R. Khenata, S. Bin-Omran,” Structural, Electronic, and Magnetic Characteristics of $Co_{1-x}Fe_xMnSb$: Insight from DFT Computation”, **Journal of Superconductivity and Novel Magnetism**, (2024).
- 61) Noorhan F. AlShaikh Mohammad ; **Mohammed S. Abu-Jafar**; Jihad H. Asad ; Mahmoud Farout ; A. Bouhemadou ; Ahmad A. Mousa ; R. Khenata; Nazia Erum ; Abdullah Chik,” FP-LAPW study of structural, magnetic, electronic, elastic, and thermoelectric properties of $CoCrS$ Half-Heusler compound”, **AIP Advances**, (2024).
- 62) Noorhan F. AlShaikh Mohammad, **Mohammed S. Abu-Jafar**, Jihad H. Asad, A. Bouhemadou, Ahmad A. Mousa, R. Khenata, and Abdullah Chik,” Investigating of structural, electronic, magnetic, dynamic, and thermoelectric

- properties of CoCrSe half-Heusler compound using FP-LAPW method”, **Eur. Phys. J. B, (2024).**
- 63) Noorhan F. AlShaikh Mohammad, **Mohammed S. Abu-Jafar**, Jihad H. Asad, A. Bouhemadou, Ahmad A. Mousa, R. Khenata, Abdullah Chik,” First-principles calculations of structural, elastic, electronic, magnetic, optical, thermoelectric, and dynamic properties of CoCrTe half-Heusler compound”, **Optical and Quantum Electronics, (2024).**
- 64) Hazem Abu-Farsakh, **Mohammed S. Abu-Jafar**, Abdallah Qteish,” Electronic structure of mono-, di- and tri-fluorides: Hybrid functional and modified Becke–Johnson potential calculations”, **Computational Materials Science, (2024).**
- 65) Rowaa S. AL-Jallad, A. Samih, R. El Fdil, Z. Fadil, **Mohammed S. Abu-Jafar**, E. Salmani, Mahmoud Farout, Chaitany Jayprakash Raorane, Ahmad A. Mousa,” DFT analysis of electronic, magnetic and elastic behavior in SmMnO₃”, **Eur. Phys. J. Plus, (2024).**
- 66) Omer Kabi, **Mohammed S. Abu-Jafar**, Mahmoud Farout, Ahmad A. Mousa, Abdelmadjid Bouhemadou, Nazia Erum, Said M. Azar, Ahmed Bassalat, Hadil Abualrob, Ahmad Y. Thabaineh, and Rabah Khenata,” Ab Initio Investigation of the Structural, Elastic, Dynamic, Electronic, And Magnetic Properties of Cubic Perovskite CeCrO₃”, **ACS Omega, (2024).**
- 67) Asif Hosen, Ahmad A. Mousa, Md. Adil Hossain, **Mohammed S. Abu-Jafar**, Redi Kristian Pingak,” Unraveling lead-free Fr-based perovskites FrQCl₃ (Q = Ca, Sr) and their pressure induced physical properties: DFT analysis for advancing optoelectronic performance”, **Journal of Physics and Chemistry of Solids, (2024).**
- 68) Rowaa S. AL-Jallad, A. Samih, **Mohammed S. Abu-Jafar**, Mahmoud Farout, R. El Fdil, Z. Fadil, E. Salmani, Chaitany Jayprakash Raorane, Ahmad A. Mous, Nazia Erum,” First-Principles investigations into electronic, magnetic, elastic, and

optical phenomena in SmCrO₃: Towards spintronic and magnetic storage applications”, **Journal of Molecular Structure**, (2024).

- 69) Sheikh Joifullah, Md. Adil Hossain, Maruf Al Yeamin, Md. Mahfuzul Haque, Redi Kristian Pingak, Noorhan F. AlShaikh Mohammad, **Mohammed S. Abu-Jafar**, Ahmad A. Mousa, Asif Hosen, ”First-principles investigation of pressure-modulated structural, electronic, mechanical, and optical characteristics of Sr₃PX₃ (X=Cl, Br) for enhanced optoelectronic application”, **Optical and Quantum Electronics**, (2024).
- 70) Md. Adil Hossaina, Asif Hosena, Heider A. Abdulhussein, Ahmad A. Mousad, Md. Muneef Hasan, Istiak Ahmed Ovi, Md. Riazul Islam, Redi Kristian Pingak, Mohammed S. Abu-Jafar, ”Investigation of the physical properties and pressure-induced band gap tuning of Sr₃ZBr₃ (Z=As, Sb) for optoelectronic and thermoelectric applications: A DFT - GGA and mBJ studies”, **Results in Engineering**, (2024).
- 71) Md. Adil Hossain, Ali A. Sabi, Heider A. Abdulhussein, Ahmad A. Mousae, Mohammed S. Abu-Jafarg, Redi Kristian Pingak, Abbas H. Abo Nasria, Waqed H. Hassan, Noorhan F. AlShaikh Mohammad, Asif Hosen, ” Insights into the pressure-dependent physical properties of cubic Ca₃MF₃ (M =As and Sb): First-principles calculations”, **Heliyon 10** (2024).
- 72) Hasan A. Masri1, Mohammed S. Abu-Jafar, Noorhan F. AlShaikh Mohammad, Saber Saad Essaoud, ” Extensive DFT study of FeMnCrGe quaternary Heusler alloy: structural, elastic, magnetic, optical and thermoelectric properties”, **Optical and Quantum Electronics** (2025).
- 73) Maruf Al Yeamin, Asif Hosena, Md. Adil Hossain, Heider A. Abdulhussein, Redi Kristian Pingak, Sheikh Joifullah, Waqed H. Hassan, Mohammed S. Abu-Jafar, Tesfaye Abebe Geleta, ” Study on pressure-induced band gap modulation and physical properties of direct band gap Ca₃NX₃ (X =Cl, Br) for optoelectronic and

thermoelectric applications”, **Surfaces and Interfaces** **56** (2025).

- 74) Heider A. Abdulhusseina, Md Adil Hossain, Asif Hosenc, Diana Dahliah, Mohammed S. Abu-Jafar, Amine Harbi, Redi Kristian Pingak, M. Moutaabbid, Istiak Ahmed Ovi, Md Riazul Islam, Md Kaab Bin Hossen,” A comprehensive analysis of the structural, phonon, electronic, mechanical, optical, and thermophysical properties of cubic Ca_3SbX_3 ($\text{X} = \text{Cl}, \text{Br}$): DFT - GGA and mBJ studies”, **Materials Science in Semiconductor Processing** **187** (2025).
- 75) Muneef Hasan, Adil Hossain, Heider A. Abdulhussein, Abdullah Al Shadi, Bijoy Sorker, Ahmed Adnan Al-Khafagi, Redi Kristian Pingak, Diana Dahliah, Mohammed S. Abu-Jafar, Asif Hosen,” A comprehensive analysis of structural, electronic, optical, mechanical, thermodynamic, and thermoelectric properties of direct band gap Sr_3BF_3 ($\text{B} = \text{As}, \text{Sb}$) photovoltaic compounds: DFT-GGA and mBJ approach”, **Inorganic Chemistry Communications** **171** (2025).
- 76) Omer Kabi, A. Samih Mahmoud Farout, R. El Fdil , E. Salmani, Z. Fadil , Nazia Erum, Mohammed S. Abu-Jafar , Seong Cheol Kim Chaitany Jayprakash Raorane, Fohad Mabood Husain, “A first-principles study of structural, electronic, magnetic, and mechanical properties in CeGaO_3 ”, **Physica B** **699** (2025).
- 77) Asif Hosen, Md. Rafiqul Islam, Ahmad A. Mousa, Mohammed S. Abu-Jafar,” A deep dive into cation-modified structural, mechanical, magneto-electronic, and thermophysical properties of MAIO_3 ($\text{M} = \text{Ca}, \text{Sr}, \text{Ba}, \text{and Ra}$): First-principles investigation”, **Results in Engineering** **25** (2025).
- 78) Hasan A. Masri, Mohammed S. Abu-Jafar, Abdelmadjid Bouhemadou, and Nadjib Baadji, “Multifunctional Properties of FeMnScAl Quaternary Heusler Alloy: Insights into Spintronics, Photovoltaics , and Thermoelectric Applications”, **J. Phys. Chem. C** **129** (2025).
- 79) Asif Hosen, Diana Dahliah, Noorhan F. AlShaikh Mohammad, Ahmad A. Mousad, Mohammed S. Abu-Jafar,” A computational study on the comparative

analysis of tetragonal complex metal hydride Q_2FeH_5 ($Q = Mg, Ca, Sr$) for hydrogen storage applications”, **International Journal of Hydrogen Energy** **102** (2025).

80) Ruba Zahi Theeb Al-Gharabah, A. Samih , R. El Fdil , Mohammed S. Abu-Jafara , Mahmoud Farout, E. Salmani , Z. Fadil, Chaitany Jayprakash Raoranec, Fohad Mabood Husaind, Ahmad A. Mousa, “First-principles investigation of structural, electronic, magnetic, elastic, and thermodynamic properties of Sc_2ZrAl full-Heusler alloy”, **Solid State Communications** **404** (2025).

81) Asif Hosena, Ebrahim Nemati-Kande, Hanof Dawas Alkhaldi, Ahmad A. Mousa , Ali Akremie, Imed Boukhris, Mohammed S. Abu-Jafar, “Designing high-capacity hydrogen storage materials: DFT insights into Ca-based complex hydrides $MCa M' H_6$ ($M = Li, Na$; $M' = Co, Rh, Ir$)”, **Journal of Materials Research and Technology** **36** (2025)

82) Asif Hosena, Ahmad A. Mousa, Ebrahim Nemati-Kande, Asif Nawaz Khan, Mohammed S. Abu-Jafar, Enrico Benassi, E.A. Elghmaz, N.S. Abd EL-Gawaad, Jihad Asad, ” Systematic computational screening and design of double perovskites Q_2LiMH_6 ($Q = K, Rb$; $M = Ga, In, Tl$) for efficient hydrogen storage: A DFT and AIMD approach”, **Surfaces and Interfaces** **67** (2025).

83) Said M. Al Azar¹, Anas Y. Al-Reyahi, Ahmad A. Mousa, Saber Saad Essaoud, Riad S. Masharfe, Ibrahim Ghabar, Nabil Al-Aqtash, Mohammed Elamin Ketfi, Mohammed S. Abu-Jafar, Emad K. Jaradat⁸, Watheq Al-Basheer, Ahmad Mufleh,” Investigation of structural, electronics, and optical characteristics of cubic $SrZr_{1-x}Ru_xO_3$ perovskites: first-principles study”, **Eur. Phys. J. Plus** **140** (2025).

XXI. Names of References:

1. Prof. Abdallah Qteish, Ph.D., Physics, Yarmouk University- Jordan

E-mail: aqteish@yu.edu.jo

2. Associate Professor Dr. Abdorrahman Abu-Labdeh, Ph.D., Physics,
Arab American University.

E-mail: alabdeh@aauj.edu

3. Prof. Ahmad Mousa, Ph.D., Physics, Basic Science Department, Middle
East University, Amman, Jordan.

E-mail: amousa@meu.edu.jo

4- Prof. Rabah Khenata, Ph.D., Physics, Laboratoire De Physique
Quantique De La Matiere et De La Modelisation Mathematique
(LPQ3M), Universite de Mascara, Mascara, Algeria.

E-mail: khenata_rabah@yahoo.fr