Curriculum Vitae

Md. Ashraf Ali, Ph.D.

BAS-Gold Medalist-2023 (Physical Sciences - Junior Group)

Professor

Department of Physics

Chittagong University of Engineering and Technology (CUET)

Chattogram -4349, Bangladesh

and

Associate Fellow, Bangladesh Academy of Sciences (BAS)

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Personal Profile:

15 Years of research and teaching experience, teaching courses at both the undergraduate and post-graduate levels. Supervised 09 M.Sc., 01 M.Phil., and 01 Ph.D. students and is currently supervising 02 Ph.D. students, 03 M.Phil. students, and 07 M.Sc. students. Published 107 articles (49-Q1/19-Q2/21-Q3) in 46 different journals with an average impact factor of 3.0^{+}. Achieving a total of 3400+ citations with an h-index of 36 and an i10-index of 75 in Google Scholar. Received the BAS-Gold Medal 2023 award, "Best Research Publication Award" for four consecutive years (2020, 2021, 2022, and 2023) from CUET. Listed in the top 2% of scientists by Stanford University, USA, and Elsevier. Maintaining collaboration with researchers from home and abroad. Serving as a peer reviewer for 60 international journals. Received research grants from the World Bank (HEAT), TWAS, UGC Bangladesh, MoST Bangladesh, DRE CUET, and Khulna University Research Cell.

Research Metrics:

Publications: 107 [First Author and/or Corresponding Author: 60]

Total Impact Factor: 347 (JCR-2024)

Google Scholar Citations: 3345+; i-10 index: 75; h-index: 36

Reviewer of Journals: 60

Students Supervision:

M.Sc.		M.Phil.		Ph.D.	
Awarded	Ongoing	Awarded	Ongoing	Awarded	Ongoing
09	07	01	03	01	02

Personal Information:

Name: Md. Ashraf Ali, *Father's name:* Late Asgar Ali, *Village:* Brammongram, *P.O.:* Kakonhat, *Upa-Zilla:* Godagari, *District:* Rajshahi, Bangladesh; *Date of Birth*: 16-11-1986; *Marital status*: Married; *Religion*: Islam; *Nationality*: Bangladeshi.

Educational Information:

Degree	Group/ Subject	Passing Year	Institution	Grade/ Class
S.S.C.	Science	2002	Pakri High School (Rajshahi Board)	A
H.S.C.	Science	2004	Rajshahi Govt. City College (Rajshahi Board)	A
B.Sc. (Hons) (4 years Integrated)	Physics	2008 (held in 2009, Result in 2010)	Rajshahi University	First Class
M.Sc. (Solid State Physics)	Physics	2009 (held in 2010, Result in 2011)	Rajshahi University	First Class
M.Phil.	Physics	2015 (12.08.2019	Chittagong University of Engineering and Technology	Awarded
Ph.D.	Physics	2019 (02.11.2019)	Chittagong University of Engineering and Technology	Awarded

Teaching Experience:

1. **11.12.2022 to till date**
   Professor, Department of Physics, Chittagong University of Engineering and Technology (CUET), Chattogram-4349, Bangladesh.

2. **18.11.2020 to 10.12.2022**
   Associate Professor, Department of Physics, Chittagong University of Engineering and Technology (CUET), Chattogram-4349, Bangladesh.

3. **20.09.2015 to 17.11.2020**
   Assistant Professor, Department of Physics, Chittagong University of Engineering and Technology (CUET), Chattogram-4349, Bangladesh.

4. **10.06.2012 to 19.09.2015**
   Lecturer, Department of Physics, Chittagong University of Engineering and Technology (CUET), Chattogram-4349, Bangladesh.

Dissertations:

M.Sc. Thesis entitled "*First principles study of tin oxides SnO_2 and SnO*" submitted to the Department of Physics, University of Rajshahi- work done as a partial fulfillment of the Master degree.

M.Phil. Thesis entitled "*Study of the structural, magnetic and electrical properties of Sn-substituted Ni-Zn ferrites*" submitted to the Department of Physics, CUET - work done as a partial fulfillment of the Master of Philosophy degree.

Ph.D. Thesis entitled "*Synthesis and characterization of Y and Sn ions substituted Mg-Zn ferrites*" submitted to the Department of Physics, CUET - work done as a partial fulfillment of the Doctor of Philosophy degree.

Awards and Honors:

1. **Member, National Young Academy of Bangladesh (NYAB).**
2. **Best oral presentation award** for Theoretical and Computational Science session at **International Conference on Electronics and Informatics-2024, held on 28-29 December 2024**, organized by the Bangladesh Electronics and Informatics Society.
3. **Awarded the best research paper award for 2023** from the Faculty of Science and Technology, CUET.
4. **Awarded BAS-Gold Medal-2023 (Physical Sciences - Junior Group) by Bangladesh Academy of Sciences (BAS),** the apex body of eminent scientists and technologists in Bangladesh.
5. **Elected Associate Fellow (2023) of the Bangladesh Academy of Sciences (BAS),** the apex body of eminent scientists and technologists in Bangladesh.
6. **Awarded the best research paper award for 2022** from the Faculty of Engineering and Technology, CUET.
7. **Awarded the best research paper award for 2021** from the Faculty of Engineering and Technology, CUET.
8. **Awarded a research grant [40,810 USD]** from **TWAS [The World Academy of Sciences]** for the development of an Advanced Computational Materials Research Laboratory (ACMRL) at the Department of Physics, CUET.
9. **Awarded the best research paper award for 2020** from the Faculty of Engineering and Technology, CUET.
10. **Awarded a research fellowship** by the Ministry of Science and Technology (MoST) for the period of 2010-2011.
11. **Awarded University Scholarship** (General) on the basis of B.Sc. (Hons.) result.
12. **Awarded Rajshahi Board Scholarship** (General) on the basis of H.S.C. result.
13. **Awarded local MP's Scholarship** (General) on the basis of S.S.C. result.

Invited/Distinct Positions:

1. **Organizing secretary,** Conference on Computational Physics and Materials Science (CCPMS-2025) hosted by the Condensed Matter Physics Lab Alumni, Department of Physics, University of Rajshahi at University of Rajshahi. The conference featured a keynote speech, two invited speeches, and a Poster session (60 posters were presented), with 160 participants in attendance.
2. **Co-Chair** at the International Conference on Electronics and Informatics-2024, organized by the Bangladesh Electronics and Informatics Society, 28-29 December 2024, Dhaka, Bangladesh.
3. **Invited Talk,** The rise of 212 MAX phase borides with enhanced thermo-mechanical properties, presented at International Conference on Advanced Materials Science & Engineering and High Tech Device Application (ICMATSE), held on 24-26 October 2024, Gazi University, Ankara, Turkiye.

4. **Invited Talk**, MAX/MAB Phases: A Family of Prospective Materials, presented at International Conference on Physics-2024, organized by Bangladesh Physical Society, 9-11 May 2024, Dhaka, Bangladesh.
5. **Co-Chair** at the International Conference on The Role of Science and Technology towards 4IR" organized by the Faculty of Science, University of Rajshahi, Bangladesh, 5-6 October 2023.
6. **Organizing secretary,** 5th international conference (5th ICPSDT-2023) hosted by the physics department at CUET. The conference featured four keynote speakers and fourteen invited speakers, with 200 participants in attendance. Twenty of those participants were from overseas and participated in the conference in person.
7. **Invited Presentation,** DFT Prediction of Stability and Physical Properties of Ti_2PB_2 Boride, presented at the Department of Physics, CUET, 2023, Chattogram, Bangladesh.
8. **Co-Chair** at 6th ICMERE-2021, organized by the Department of Mechanical Engineering, CUET, 12-13 December 2021, Chattogram, Bangladesh.

List of Publications:

[Bold letters indicate Dr. Ali; *Indicates corresponding authorship; Citations: 3345+ h-index: 36, i10 index: 75; Cumulative Impact Factor (JCR-2024) ~349]

1. S.H. Sakib; Shariful Islam; M. Nasir Uddin; A.K.M Naim Ishtiaq; M.R. Rana; N.A. Roktim; **M. A. Ali***; M.E. Hossain, K. Hoque, *A DFT Study to Investigate the Stability and Physical Features of Y_2AB MAX Phase Boride*, **Submitted**.

2. M.I. Naher, M. Montasir, M.Y.H. Khan, **M. A. Ali**, M.M. Hossain, M.M. Uddin, M.Z. Hasan, M.A. Hadi, S.H. Naqib, *Investigation of the Pressure Dependent Physical Properties of MAX Phase Ti_2AlX (X = B, C, and N) Compounds: A First-Principles Study*, **Submitted**.

3. Md Nasir Uddin, A. K. M Naim Ishtiaq, Shariful Islam, Md. Rasel Rana, Noor Afsary, Karimul Hoque, **Md. Ashraf Ali***, *DFT insights into new Boron-based MAX phases, M_3GaB_4 [M = Hf, Zr, Ta] and 2D derivatives, MXenes M_3B_4 [M = Hf, Zr, Ta], for high-temperature and energy storage applications*, **Submitted**.

4. M. A. Rayhan, M. M. Hossain, M. M. Uddin, S. H. Naqib, **M. A Ali*,** *DFT exploration of novel direct band gap semiconducting halide double perovskites, $A_2AgIrCl_6$ (A = Cs, Rb, K), for solar cells application*, **Submitted**.

5. Md. Rasidul Islam, Ovijit Das, **M. A. Ali**, Asif Abdullah Khan, Dayan Ban, Density function theory analysis of the physical properties of $Pb_{10}(PO_4)_6(OH)_2$(K99) material, **Submitted.**

6. Sonet Kumar Saha, **Md. Ashraf Ali***, A. K. M. Akther Hossain, *Study of the structural, dielectric properties and AC conductivity of $Bi_{1-x}Y_xFe_{0.7}Mn_{0.3}O_3$ ceramics*, **Submitted**.

7. Yeasir Ahmed, Md Rasadujjaman, Md Didarul Islam Bhuyan, Md Hazrat Ali, Md Rezaul Karim, Md Sahab Uddin, Abu Talib Md Kaosar Jamil, Syed Jamal Ahmed, **Md Ashraf Ali**, Md Anwar Hossain, *Annealing temperature effect on the optical properties of spin–coated Ru–doped NiO films*, **Optical Materials** 167 (2025) 117345.

8. M. M. Rabbi, M. H. Mia, S. S. Saif, U. Ahmed, M. M. Hossain, M. M. Uddin, **M. A. Ali***, *DFT Prediction of Double Perovskites $A_2B'RhCl_6$ (A = Cs, Rb; B' = Na, K) for Green Energy Technology*, **Computational Condensed Matter** 44 (2025) e01093**.**

9. J. K. Rony, S. Nath, N. Jahan, M. M. Hossain, M. M. Uddin, **M. A. Ali***, *DFT prediction of new MAX phase borides: Ta_2AB [A = P, Zn, Ge, Cd, Tl]*, **Inorganic Chemistry Communications** 180 (2025) 115076.

10. A. K. M Naim Ishtiaq, Md Nasir Uddin, Md. Rasel Rana, Shariful Islam, Noor Afsary, Karimul Hoque, **Md. Ashraf Ali*,** *Exploration of new 212 MAX phases: M_2AB_2 (M=Mo, Ta; A=Ga, Ge) via DFT calculations*, **Advanced Theory and Simulations** (2025) 2401448.

11. U. Ahmed, H. Akter, A. Hossain, M.M. Hossain, M.M. Uddin, S. H. Naqib, A. K. M. A. Islam, **M. A. Ali***, *Anion (S) substitution as a pathway for tuning the physical properties of $CsTaO_3$*, **New Journal of Chemistry** 49 (2025) 7682-7699.

12. N. Jahan, **M.A. Ali**, M. M. Hossain, R. Hasan, S. Akhter, M.N. I. Khan, M. M. Uddin, *A comprehensive study of RE ions Ho doped Ni-Zn nanoferrites synthesized by sol-gel auto-combustion techniques*, **Journal of Magnetism and Magnetic Materials** 624 (2025) 173042.

13. Aslam Hossain, Md. Mukter Hossain, Hasina Akter, Md. Mohi Uddin, **Md. Ashraf Ali,** Saleh Hasan Naqib, *Ultralow lattice thermal conductivity with outstanding figure of merit of newly predicted Zintl phases: XIn_2C_2 (X = Sr, Ba)*, **ACS Applied Energy Materials** 8 (2025) 5092–5109.

14. M. H. Mia, U. Ahmed, S. K. Saha, M. A. Ali*, *Unveiling Mechanical, Electronic, and Optical Properties of Newly Synthesized Mo_2VAlC_2 and $Mo_2V_2AlC_3$ o-MAX Phases via First-Principles Calculations*, **Journal of Materials Research and Technology** 36 (2025) 2468-2484.

15. M. Z. Hasan; M. H. Haque; **M. A. Ali**; M. M. Hossain; M. M. Uddin, *Structural, optical, and photocatalytic efficacy of Ti_3C_2 and M_2C (M=Ti, V, Cr, Nb) MXene materials synthesized by etching technique*, **AIP Advances** 15 (2025) 035334.

16. S. Mahmud, Usama Ahmed, M.A.U.Z. Atik, Md. Mukter Hossain, M. Uddin and **M. A. Ali*,** *Novel $Cs_2AuIMIIIF_6$ (M = As, Sb) double halide perovskites: sunlight and industrial wasted heat management device applications*, **Physical Chemistry Chemical Physics** 27 (2025) 4686.

17. **M. A. Ali*,** S. Nath, S. Mahmud, N. Jahan, M. M. Uddin, *MAX phase borides, the potential alternative of well-known MAX phase carbides: a case study of V_2AB [A = Ge, P, Tl, Zn] via DFT method*, **Diamond & Related Materials** 150 (2024) 111668.

18. Noor Afsary, Md Nasir Uddin, A. K. M Naim Ishtiaq, Md Koushik Alam, **Md. Ashraf Ali**, Karimul Hoque, Md Omar Faruk Rasel, *First-principal analysis and design of $TaPO_5$-based waveguides for photonic circuitry* **Physica B** 696 (2024) 416645.

19. Noor Afsary, Md Nasir Uddin, Shariful Islam, Md Koushik Alam, **Md. Ashraf Ali**, Karimul Hoque, Md Omar Faruk Rasel, *Elevating NIR Photonic Integration with Tantalum-Niobium Pentoxide,* **Physica Scripta** 99 (2024) 115972.

20. M. M. Uddin, M. Z. Hossain, M. H. Kabir, Swarup Ghosh, M. H. Haque, M. M. Hossain, **M. A. Ali**, Md. Akhtaruzzaman, Abdulaziz M. Alanazi, S. Mondal, Joydeep Chowdhury, D. Karmakar, and Debnarayan Jana; *Synergistic Effects of Rare-Earth Ions (Ho, Yb) Doped on the Photo-Catalytic Efficacy of V_2O_5 for Removal of Pollutants from Industrial Waste Water* **Heliyon** 10 (2024) e37689.

21. S. Mahmud, M. M. Hossain, M. M. Uddin, **M. A. Ali*,** *Prediction of X_2AuYZ_6 (X = Cs, Rb; Z = Cl, Br, I) double halide perovskites for photovoltaic and wasted heat management device applications,* **Journal of Physics and Chemistry of Solids** 196 (2025) 112298.

22. Md. Ferdous Rahman, Md. Abul Bashar Shanto, **Md. Ashraf Ali**, Latha Marasamy, Abdellah Benami, Aijaz Rasool Chaudhry, Ahmad Irfan, *A new exploration of the impact of different wide-bandgap S-chalcogenides Electron Transport Layers (ETL) on the performance of BaSi2-based solar cells,* **Emergent Materials** (2024).

23. Ruma Akther, N. Jahan, **M. A. Ali***, *Study of New MAX Phase Materials: Sc_2AX (A= Bi, Br; X=C, N, B) via Ab-initio Method* **Materials Today Communications** 40 (2024) 109679.

24. A. K. M Naim Ishtiaq, Md Nasir Uddin, Noor Afsary, Md Koushik Alam, **Md. Ashraf Ali***, Karimul Hoque, *A DFT approach to investigate the electronic, mechanical, and optical properties of M_3GaB_2 (M = Ti, Hf) 312 MAX Phases,* **Heliyon** 10 (2024) e33651.

25. M. Biswas, S. Ghosh, J. Chowdhury, **M. A. Ali,** M. M. Hossain, S. H. Naqib, and M. M. Uddin, *An inclusive study of lead-free perovskite $CsMI_3$ materials for photovoltaic and optoelectronic appliance explored by a first principles study,* **Materials Today Communications** 40 (2024) 109422.

26. M.R. Rana, S. Islam, K. Hoque, S. Mahmud, **M. A. Ali***, *Newly synthesized Pb-based 312 MAX phases M_3PbC_2 (M=Zr and Hf): A First-principles study,* **Diamond & Related Materials** 146 (2024) 111245.

27. S. Islam, M.R. Rana, Prima Das, K. Hoque, S.H. Naqib, **M. A. Ali***, *DFT insights into i-MAB phase, $Mo_4Y_2Al_3B_6$: a potential thermal barrier coating and solar heat reducing material,* **Physica Scripta** 99 (2024) 055975.

28. M. A. Rayhan, **M. A. Ali***, N. Jahan, M. M. Hossain, M. M. Uddin, A. K. M. A. Islam, S. H. Naqib, *Insights into the unrevealed physical properties of $Sc_2Al_2C_3$ compared with other Sc-Al-C systems via ab-initio investigation*, **Physics Open** 19 (2024) 100217.

29. H. Akter, M. M. Hossain, M. M. Uddin, S. H. Naqib, **M. A. Ali***, *Effects of S substitution on the structural, optoelectronic, and thermomechanical properties of $KTaO_3$ through density functional theory*, **Journal of Physics and Chemistry of Solids** 190 (2024) 112021.

30. S. Islam, R. Ahmad, **M. A. Ali**, M. M. Hossain, M. M. Uddin, S. H. Naqib, *Ab-initio insights into the physical properties of XIr_3 (X = La, Th) superconductors: A comparative analysis*, **Results in Materials** 22 (2024) 100568.

31. H. Akter, **M. A. Ali***, M. M. Hossain, M. M. Uddin, S. H. Naqib, *Oxysulfide Perovskites: Reduction of the Electronic Band Gap of $RbTaO_3$ by Sulfur Substitution*, **Physica Scripta** 99 (2024) 045950.

32. Md Nasir Uddin; A. K. M Naim Ishtiaq; Shariful Islam; Md. Rasel Rana; **Md. Ashraf Ali***, Karimul Hoque, *Prediction of new 212 M_2AB_2 borides as a promising candidate for future engineering: DFT calculations,* **Materials Today Communications** 39 (2024) 108536.

33. M. N. Hossain, M. M. Rahman, **M. A. Ali**, N. Jahan, A. A. Momin, M. M. Rahman, M. A. Hakim, *Novel Gadolinium (Gd) and Chromium (Cr) Co-Doped Yttrium Iron Garnet ($Y_3Fe_5O_{12}$) Nanoparticles,* **Arabian Journal for Science and Engineering** 49 (2024) 9967–9982.

34. A. Hossain, **M. A. Ali**, M.M. Uddin, S.H. Naqib, M.M. Hossain, *Theoretical studies on phase stability, electronic, optical, mechanical and thermal properties of chalcopyrite semiconductors $HgXN_2$ (X=Si, Ge and Sn): A comprehensive DFT analysis,* **Materials Science in Semiconductor Processing** 172 (2024) 108092.

35. Razu Ahmed, Md Sajidul Islam, M.M. Hossain, **M. A. Ali**, M.M. Uddin, S. H. Naqib, *A comprehensive first-principles insights into the physical properties of binary intermetallic Zr_3Ir compound*, **Results in Materials** 21 (2024) 100518.

36. S. Mahmud, **M. A. Ali***, M.M. Hossain, M.M. Uddin, *DFT aided prediction of phase stability, optoelectronic and thermoelectric properties of A_2AuScX_6 (A= Cs, Rb; X= Cl, Br, I) double perovskites for energy harvesting technology*, **Vacuum** 221 (2024) 112926.

37. M. H. Kabir; M. Z. Hossain; M. A. Jalil; M.M. Hossain; **M. A. Ali**; M.M. Uddin; D. Jana; M. M. Rahman; M. K. Hossain; K. S. Al-mugren, *Enhancement of the photocatalytic performance of V_2O_5 by rare-earth ions doping, synthesized by facile hydrothermal technique,* **Optical Materials** 147 (2024) 114724.

38. Md. Mohi Uddin, Mohammad Humaun Kabir, **Md. Ashraf Ali**, Md. Mukter Hossain, Mayeen Uddin Khandaker, Sumit Mandal, A. Arifutzzaman, Debnarayan Jana,

Graphene-like Emerging 2D Materials: Recent Progress, Challenges and Future Outlook, **RSC Advances** 13 (2023) 33336.

39. Md. Rasidul Islam, Abu Zahid, M Atikur Rahman, Md. Ferdous Rahman, M. A. Islam, M. Khalid Hossain, **M. A. Ali**, Muhammad Aamir Iqbal, FarhadIlahi Bakhsh, and Sohail Ahmad; *Tuning the optical, electronic, and mechanical properties of inorganic Ca_3PCl_3 perovskite via biaxial strain*, **Journal of Physics and Chemistry of solids** 184 (2024) 111722.

40. Md. Ferdous Rahman, Md. Harun-Or-Rashid, Md. Rasidul Islam, Avijit Ghosh, M. Khalid Hossain, Mustafa K. A. Mohammed, Sagar Bhattarai, Rahul Pandey, Jaya Madan, **M. A. Ali**, *Exploring the Impact of Strain on the Electronic and Optical Properties of Inorganic Novel Cubic Perovskite Sr_3PI_3*, **Physica Scripta** 98 (2023) 115105.

41. J. Islam, M. D. Islam, **M. A. Ali***, H. Akter, A. Hossain, M. Biswas, M. M. Hossain, M. M. Uddin, S. H. Naqib, *DFT insights into MAX phase borides Hf_2AB [A = S, Se, Te] in comparison with MAX phase carbides Hf_2AC [A = S, Se, Te]*, **ACS Omega** 8 (2023) 32917-32930.

42. F. Rahman, M. M. Ali, **M. A. Ali**, M. M. Uddin, S. H. Naqib, M. M. Hossain; *DFT approach into the physical properties of MTe_3 (M = Hf, Zr) superconductors: a comprehensive study;* **AIP Advances** 13 (2023) 085126**.**

43. S. Islam, M. R. Rana, M. K. Hoque, G. G. Biswas, M. E. Hossain, M. M. Hossain, M. M. Uddin, S. H. Naqib, **M. A. Ali*,** *A comprehensive exploration of the physical properties of M_2GaB (M = Ti, Zr, Mo, Hf) through DFT method*, **Results in Materials** 19 (2023) 100438.

44. Shazzad Hossain, Md Emran Hossain, Shariful Islam, Md Rasel Rana, G.G. Biswas, **Md Ashraf Ali*,** K. Hoque, M.N.I. Khan, *Synthesis of Sr-doped $Ni_{0.5}Zn_{0.5}Sr_xFe_{2-x}O_4$ and the study of its structural, mechanical, magnetic, and electrical properties for high-frequency applications*, **Physics Open** 17 (2023) 100172.

45. Atanu Sarker Jyoti, G. G. Biswas, Md. Rasel Rana, Shariful Islam, Md. Emran Hossain, M. N. I. Khan, K. Hoque, **Md. Ashraf Ali***, *Investigation of the Structural, Electrical and Magnetic Properties of Vanadium Substituted Mn-Zn Ferrites*, **Discover Materials** 3 (2023) 20.

46. M. I. Naher, **M. A. Ali**, M. M. Hossain, M. M. Uddin, S. H. Naqib, *A comprehensive ab-initio insights into the pressure-dependent mechanical, phonon, bonding, electronic, optical, and thermal properties of CsV_3Sb_5 Kagome compound*, **Results in Physics** 51 (2023) 106742.

47. M. H. Kabir, M. H. Hossain, **M.A. Ali**, M.M. Uddin, M.L. Ali, M. Z. Hasan, A.K. M. A Islam, S.H. Naqib, *First-principles study of mechanical, thermal, electronic, optical and superconducting properties of C40-type germanide-based MGe_2 (M = V, Nb and Ta)*, **Results in Physics** 51 (2023) 106701**.**

48. M. Sohel, M. M. Uddin, **M. A. Ali**, Md Mukter Hossain, A. K. M. A. Islam, S. H. Naqib *Impact of M atomic species on physical properties of M_2TlC (M= Ti, Zr, Hf): a first principle calculations,* **AIP Advances** 13 (2023) 065209.

49. M. R. Rana, S. Islam, M. K. Hoque, G. G. Biswas, M. E. Hossain, S. H. Naqib, **M. A. Ali***, *DFT prediction of the stability and physical properties of M_2GaB (M = Sc, V, Nb, Ta),* **Journal of Materials Research and Technology** 24 (2023) 7795-7815.

50. Gokhan Surucu, Aysenur Gencer, Ozge Surucu, **Md. Ashraf Ali**, *DFT insights into noble gold-based compound, Li_5AuP_2: effect of pressure on physical properties,* **ACS Omega** 8 (2023) 15673–15683.

51. Mehnaj Akhter, Md. Shamim Ahasan, **M. A. Ali***, F. Parvin; *Elastic, electronic, optical and thermodynamic properties of M_2SeC (M= Hf, Zr) under high pressure;* **AIP Advances** 13 (2023) 025154.

52. Prima Das, N. Jahan, **M. A. Ali***, *DFT insights into Nb-based 211 MAX phase Carbides: Nb_2AC (A= Ga, Ge, Tl, Zn, P, In, Cd),* **RSC Advances** 13 (2023) 5538.

53. **M. A. Ali***, M. M. Hossain, M. M. Uddin, A. K. M. A. Islam, S. H. Naqib, *The rise of 212 MAX phase borides: DFT insights into the physical properties of Ti_2PB_2, Zr_2PbB_2, and Nb_2AB_2 [A = P, S] for thermo-mechanical applications,* **ACS Omega** 8 (2023) 954.

54. M. S. Hossain, N. Jahan, M. M. Hossain, M. M. Uddin, **M. A. Ali***, *High pressure mediated physical properties of Hf_2AB (A = Pb, Bi) via DFT calculations,* **Materials Today Communications** 34 (2023) 105147.

55. Rafiqul Islam, M. M. Hossain, **M. A. Ali**, M. M. Uddin, S. H. Naqib, *Metallicboro-carbides of A_2BC (A=Ti, Zr, Hf and W): A comprehensive theoretical study for thermo-mechanical and optoelectronic applications*; **RSC Advances** 12 (2022) 32994.

56. J. Islam, S. K. Mitro, M. M. Hossain, M. M. Uddin, N. Jahan, A. K. M. A. Islam, S. H. Naqib, **M. A. Ali***, *Exploration of physical properties of newly synthesized Kagome superconductor $LaIr_3Ga_2$ using different exchange correlation functionals*, **Physical Chemistry Chemical Physics** 24 (2022) 29640.

57. M.A. Hadi, Istiak Ahmed, **M.A. Ali**, M.M. Hossain, M.T. Nasir, M.L. Ali, S.H. Naqib, A.K.M.A. Islam, *A comparative DFT exploration on M- and A-site double transition metal MAX phase, Ti_3ZnC_2*; **Open Ceramics** 12 (2022) 100308.

58. Md. Atikur Rahman, Ibrahim Kholil, Rukaia Khatun, Sushmita Sarker, Mahbub Hasan, **M. A. Ali**, Md. Zahidur Rahaman, Khandaker Monower Hossain, Md. Zahid Hasan, *High pressure study of new type of MAX phases: Hf_2AB_2 (A = In, Sn),* **Physica Status Solidi B** 260 (2022) 202200102.

59. Muhammad Waqas Qureshi, **M. A. Ali**. Xinxin Ma, Guangze Tang, M. Usman Javed, Durga Paudyal, *Verification of stability and unraveling the electronic and physical*

properties of bulk and (001)-surfaces of newly synthesized Ti_2ZnX (X = C, N) MAX phases, **Surfaces and Interfaces** 31(2022) 102032.

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82. **M. A. Ali***, S. H Naqib, *Recently synthesized* $(Ti_{1-x}Mo_x)_2AlC$ *(*$0 \leq x \leq 0.20$*) solid solutions: deciphering the structural, electronic, mechanical and thermodynamic properties via ab initio simulations,* **RSC Advances** 10 (2020) 31535.

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109. **M. A. Ali***, N. Jahan, A. K. M. A. Islam; *Sulvanite compounds Cu_3TMS_4 (TM= V, Nb and Ta): elastic, electronic, optical and thermal properties using first-principles method*; **Journal of Scientific Research** 6 (2014) 407-419.

110. N. Jahan, **M. A. Ali**; *A theoretical study of elastic, electronic, optical and thermodynamic properties of AlB_2 and TaB_2*; **Bangladesh Journal of Physics** 15 (2014) 93-103.

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Research Projects:

Sl No	Role	Title	Funding Organization	Duration	Amount
1.	ASPM	Establishment of Advanced Materials Research Laboratory for	**World Bank (HEAT-UGC)**	July 2025-June 2028	55743000.0 BDT

		Energy Storage Capacity Enhancement			
2.	Co-Principal Investigator	Development of New MXene-based Anode Materials for Li-ion Batteries from 312 MAX Phases [M = Hf, Mo, Mo, Ta; A = Ha, Ge; X = N]: A Computational Study	**Khulna University Research and Innovation Centre**	2025- 2026	400000.0 BDT
3.	Principal Investigator	Searching of New MAX phases for thermal barrier coating applications through DFT calculations	**MoST, Bangladesh**	01.07.2024 – 30.06.2025	182000.0 BDT
4.	Principal Investigator	Tuning the Physical Properties of Oxide Perovskites through S Substitution: $ABO_{3-x}S_x$ (A = Ba, Ca; B = Ti, V)	**CUET DRE**	21.01.2025 – 20.01.2026	174000.0 BDT
5.	Principal Investigator	DFT Prediction of Double Perovskites $A_2B'B''Cl_6$ [A = Cs/Rb; B′ = Na/K; B″=Au/Rh] for Green Energy Technology	**CUET DRE**	01.02.2024 – 31.01.2025	214000.0 BDT
6.	Principal Investigator	Prediction of the M_2AB [M=V, Nb, Ta; A=Ge, Tl, P, Zn, Cd, Cu] borides by the DFT method	**UGC, Bangladesh**	01.01.2024 – 31.12.2024	212000.0 BDT
7.	Co-Principal Investigator	Exploring the stability and Physical properties of M_2AX [M = Ti,Zr, Hf; A=Ge, Tl, P, Zn, Cd, Cu; X = C/B] phases: a DFT study	**Khulna University Research and Innovation Centre**	2023- 2024	300000.0 BDT
8.	Principal Investigator	Synthesis and study of the photo-catalytic activity of R_2CrFeO_6 [R = Y, La] for the degradation of organic dyes	**MoST, Bangladesh**	01.07.2023 – 30.06.2024 (**Completed**)	250000.0 BDT
9.	Principal Investigator	Development of an Advanced Computational Materials Research Laboratory	**TWAS**	03/11/2021-31/12/2023 (**Completed**)	40810.0 USD
10.	Co-Principal Investigator	First principles analysis of Y-based 211 M2AX compounds (M = transition metals, A = main group elements, X = C/N)	**Khulna University Research Cell**	October 2022-October 2023 (**Completed**)	200000.0 BDT
11.	Project member	Study of photocatalytic behavior of recently synthesized high-quality V_2O_5 by hydrothermal technique for wastewater treatment	**UGC, Bangladesh**	01/05/2022-30/04/2023 (**Completed**)	298400.0 BDT

12.	Principal Investigator	"First-principles study of 211 MAX phase carbides: Nb_2AC (A = P, Zn, Ga, Ge, Cd, In, Tl)"	**MoST, Bangladesh**	01/07/2021-30/06/2022 (**Completed**)	200000.0 BDT
13.	Co-Principal Investigator	First principles study of 211 MAX phase borides (M = Transition metal, A = Al/Ga, X = B)	**Khulna University Research Cell**	October 2021-October 2022 (**Completed**)	200000.0 BDT
14.	Project member	Synthesis and characterization of 2D transition metal carbides (MXenes, Ti_2C and Ti_3C_2): A theoretical and an experimental approach	**CUET DRE**	2021-2023 (**Completed**)	450000.0 BDT
15.	Project Student	Synthesis and characterization of Y and Sn ions substituted Mg-Zn ferrites	**CUET DRE**	July 2017 - June 2019 (**Completed**)	450000.0 BDT
16.	Project member	Study of Ni-Sn-Zn nano ferrites for high frequency electronics applications	**CUET DRE**	July 2014 – June 2016 (**Completed**)	300000.0 BDT

Students Supervision

Sl No.	Name	Identity	Level	Status
1.	Md. Abu Rayhan	20PPHY002P	Ph.D.	Ongoing
2.	***Shuib Mahmud***	***20PPHY003P***	***Ph.D.***	***Awarded 2025***
3.	Kohinur Begum	21MPHY007P	M.Phil.	Ongoing
4.	Ruma Das	21MPHY006P	M.Phil.	Ongoing
5.	Santosh Kumar Datta	18MPHY004F	M.Phil.	Ongoing
6.	***Siyara Bibi***	***15MPHY005P***	***M.Phil.***	***Awarded 2024***
7.	Syed Saifulla Saif	22MSPHY101	M.Sc.	Ongoing
8.	Mohammed Ispat Alam Tanim	22MSPHY009	M.Sc.	Ongoing
9.	Shrabonti Nath	22MSPHY008	M.Sc.	Ongoing
10.	***Md. Nasir Uddin***	***M.S. 201710 (Khulna University)***	***M.Sc.***	***Awarded 2025***
11.	***Labib H. K. Adnan***	***MS 241720 (Khulna University)***	***M.Sc.***	***Awarded 2025***
12.	***Md. Navid Anjum Roktim***	***MS – 231709 (Khulna University)***	***M.Sc.***	***Awarded 2024***
13.	***Shahadat Hossen Sakib***	***MS 231703***	***M.Sc.***	***Awarded 2024***

		(Khulna University)		
14.	***Hasina Akter***	***20MSPHY002F***	***M.Sc.***	***Awarded 2024***
15.	***Prima Das***	***19MSPHY001F***	***M.Sc.***	***Awarded 2023***
16.	***Md. Rasel Rana***	***M.Sc.-201711 (Khulna University)***	***M.Sc.***	***Awarded 2023***
17.	***Md. Shariful Islam***	***M.Sc.-201702 (Khulna University)***	***M.Sc.***	***Awarded 2023***
18.	***Md. Sumon Hossain***	***18MSPHY004F***	***M.Sc.***	***Awarded 2022***

Reviewer:

1. ACS Applied Engineering Materials (**ACS**)
2. ACS Omega (**ACS**)
3. Advances in Materials Science and Engineering (**Hindawi**)
4. Applied Physics A (**Springer**)
5. Canadian Journal of Physics (**Canadian Science Publishing**)
6. Chinese Physics B (**IOP Science**)
7. Chemistry Select (**Wiley**)
8. Chemical Physics (**Elsevier**)
9. Ceramic International (**Elsevier**)
10. Construction and Building Materials (**Elsevier**)
11. Colloids and Interfaces (**MDPI**)
12. Diamond and related materials (**Elsevier**)
13. Energy storage (**Wiley**)
14. Emergent Materials (**Springer**)
15. Europhysics Letters (**Springer**)
16. Engineering and Technology Journal (**University of Technology-Iraq**)
17. ECS journal of solid state science and technology (**IOP Science**)
18. Heliyon (**Elsevier**)
19. High Temperature Materials and Processes (**De Gruyter**)
20. Indian Journal of Physics (**Springer**)
21. International Journal of Modern Physics B (**World Scientific**)

22. International Journal of Energy Research (**Wiley**)
23. IEEE Transactions on Nanotechnology (**IEEE**)
24. International journal of quantum chemistry (**Wiley**)
25. Journal of Alloys and Compounds (**Elsevier**)
26. Journal of the American Ceramic Society (**Wiley**)
27. Journal of the American Chemical Society (ACS)
28. Journal of Energy Storage (**Elsevier**)
29. Journal of Materials Research and Technology (**Elsevier**)
30. Journal of Materials Chemistry A (**RSC**)
31. Journal of Materials Chemistry C (**RSC**)
32. Journal of Materials Science (**Springer**)
33. Journal of Materials Engineering and Performance (**Springer**)
34. Journal of Nanoelectronics and Optoelectronics
35. Journal of Physics and Chemistry of Solids (**Elsevier**)
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44. Modern Physics Letters B (**World Scientific**)
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47. Optical and Quantum Electronics (OQEL) (**Springer**)
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59. Surfaces and Interfaces (**Elsevier**)
60. Scientific Reports (**Springer Nature**)
61. SCIENCE CHINA Materials (**Springer Nature**)
62. The Journal of physics and chemistry of solids (**Elsevier**)
63. Turkish Journal of Chemistry
64. Vacuum (**Elsevier**)

Research Experience:

1. **Jan 2010 to March 2011**
   M. Sc.thesis work - for partial fulfillment of Master's degree.
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2. **March 2011 to June 2012**
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3. **June 2013 to August 2015**
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   Supervisor: Dr. Md. Mohi Uddin, Professor, Department of Physics, Chittagong University of Engineering and Technology, Bangladesh.
4. **August 2015 to November 2019**
   Ph.D. Thesis work - for partial fulfillment of Ph.D. degree.
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5. **November 2019 to present, My duties involve:**
   1. Teaching undergraduate and postgraduate students.
   2. Supervising postgraduate students.
   3. Researching various materials of interest.

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3.**Dr. A. K. M. Abdul Hakim** (Visiting Professor, Bangladesh University of Engineering and Technology (BUET), **Bangladesh**).

4.**Dr. A. K. M. Akhter Hossain** (Professor of Physics, Bangladesh University of Engineering & Technology (BUET), Dhaka, **Bangladesh**).

5.**Dr. Saleh Hasan Naqib** (Professor of Physics, University of Rajshahi, **Bangladesh**).

6. **Dr. Md. Mohi Uddin** (Professor of Physics, Chittagong University of Engineering & Technology (CUET), Chittagong, **Bangladesh**).
7. **Dr. Sheikh Manjura Hoque** (Chief Scientific Officer, Materials Science Division, Atomic Energy Centre, Dhaka, **Bangladesh**).
8. **Dr. Md. Nazrul Islam Khan** (Chief Scientific Officer, Materials Science Division, Atomic Energy Centre, Dhaka, **Bangladesh**).
9. **Dr. Md. Anwar Hossain** (Professor of Physics, Department of Physics, Mawlana Bhashani Science and Technology University, **Bangladesh**).
10. **Dr. Md. Mukter Hossain** (Associate Professor of Physics, Chittagong University of Engineering and Technology, **Bangladesh**).
11. **Dr. A. T. M. Kaoser Jamil** (Professor of Physics, Dhaka University of Engineering & Technology (DUET), Gazipur, **Bangladesh**).
12. **Md. Abdul Hadi** (Department of Physics, University of Rajshahi, **Bangladesh**).
13. **M. Roknuzzaman** (Post Doc. Research Scholar, The University of Sydney, **Australia**).
14. **Dr. K. Ostrikov** (Professor of Physics, Queensland University of Technology and Commonwealth Scientific and Industrial Research Organization, **Australia**).
15. **Dr. Jose Alarco** (Professorial Fellow, Institute for Future Environments, Queensland University of Technology, **Australia**).
16. **Dr. Debnarayan Jana** (Professor of Physics, University Calcutta, Kolkata, **India**)
17. **Dr. Isao Tanaka** (Professor, Center for Crystal Science and Technology, University of Yamanashi, **Japan**)
18. **Dr. Satoshi Watauchi** (Professor, Center for Crystal Science and Technology, University of Yamanashi, **Japan**)
19. **Dr. Masanori Nagao** (Professor, Center for Crystal Science and Technology, University of Yamanashi, **Japan**)
20. **Dr. Xinxin Ma** (Professor, Harbin Institute of Technology, Harbin 150001, **China**)
21. **Dr. Muhammad Waqas Quresh** (University of Wisconsin-Madison, Madison, WI, **USA**)
22. **Dr. Gokhan Surucu** (Associate Professor, Gazi University, **Turkey**)
23. **Dr. Md. Akhtaruzzaman** (Professor, Islamic University of Madinah, **Saudi Arabia**)

Main Topics Taught:

Physical Optics: Interference of light, Diffraction of light, Polarization of light.

Properties of Matter: Elasticity, Surface Tension of water and mercury, Hydrodynamics, Viscosity.

Modern Physics: Special Theory of Relativity, Photoelectric Effect, Compton Effect, de Broglie Wave, Bohr's Postulates, Wave Mechanics.

Nuclear Physics: Radioactivity, Nuclear Reactions, Reactor Physics, etc.
Waves and Oscillations: Vibrations and Oscillations, Damped Vibration, Forced Vibration, Wave Motion, Sound Waves, Acoustics.
Heat and Thermodynamics: Heat, Hygrometry, Heat Radiation, Measurement of temperatures, Transmission of heat, Laws of thermodynamics.
Solid State Physics: States of matter, Crystallography, X-rays, Crystal defects, bonding in solids, Band theory, Magnetism.
Materials Science: Introduction to Materials Science, Characterization Methods of Materials, Ceramic and Bioceramic Materials, Magnetic Materials.
Condensed Matter Physics: Band theory of solids, Thermal, optical, magnetic, and dielectric properties of solids.
Experimental Techniques in Solid State Physics: Synthesis techniques: Solid state reaction, sol-gel, and hydrothermal techniques, Characterization: XRD, SEM; Magnetic, Mechanical, and Optical properties of solids.
Nano Physics: Basic Properties of Nanoparticles, Synthesis Techniques of Nanostructured Materials, Physics of Nanomaterials Characterizations.
Research Methodology: Introduction to Research, Various Stages of Research, Report/Thesis/Article Writing.

Administrative/Professional Experience:

Post	Institution/organization	Duration
Member	**Academic Council, CUET**	18.11.2020 to till date
Member	Academic Committee for Post-graduate Studies (ACPGS), **Department of Physics, CUET**	April 2019 to till date
Member	Academic Committee for Post-graduate Studies (ACPGS), **Department of ETE, CUET**	July 2019 to 2022
Associate Fellow	Bangladesh Academy of Sciences (BAS)	June 2024 to till date
Member	National Young Academy of Bangladesh (NYAB)	January 2025 to till date
Member Secretary	Conference on Computational Physics and Materials Science (CCPMS-2025)	20th April 2025
Member Secretary	5th International Conference on "Physics for Sustainable Development and Technology" (5th ICPSDT-2023)	7-8 September 2023
Tresurer	4th International Conference on "Physics for Sustainable Development and Technology" (4th ICPSDT-2023)	22-23 January 2022
Assistant Provost	Bangabandhu Hall, CUET	27.02.2017to 28.02.2018
Assistant Provost	Shaheed Tareq Huda Hall, CUET	10.11.2014 to 31.12.2016

Member	Steering committee, International Journal of Integrated Sciences &Technology (IJIST) published by the Faculty of Engineering & Technology, CUET.	2014-2016
External Examiner	Pabna University of Science and Technology (PUST), Pabna	2015

Notable Professional Society Involvements:

1. Life Member, Bangladesh Physical Society
2. Life Member, Physics Alumni Association of Rajshahi University

Language Proficiency:

Considerably good both in written and spoken English. The medium of instruction was English at the Bachelor of Science (Honors), Master of Science, Master of Philosophy, and Doctor of Philosophy levels.

Experimental Skills:

(i)Materials Synthesis Techniques: Solid-state Reaction techniques and Sol-gel process;
(ii) Measurement Techniques: Structural, Electrical, and Magnetic Properties.

Analysis Techniques and Computer Software:

Windows-based application software like MS-Word, Excel, PowerPoint, Microsoft Word 2007; Plotting software: Sigma Plot and Origin Lab; Simulation software: CASTEP code; Data analysis: XRD, FTIR, EDS, Dielectric behavior, VSM, Permeability, UV data.

References:

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2. **Prof. Saleh Hasan Naqib**
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   Tel.: +8801715049589
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3. **Prof. Md. Mohi Uddin**
   Department of Physics, CUET, Chittagong-4349, Bangladesh
   Tel.: +8801857873871
   E-mail: mohi@cuet.ac.bd

I do hereby declare that all the above information is true and correctly describes my qualifications and myself to the best of my knowledge.

Date: June 2025 (Prof. Md. Ashraf Ali, PhD)