Dr. Mohammad Abdur Rashid

CONTACT INFORMATION

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PROFESSIONAL EXPERIENCES

Assistant Professor (November 2018 – Present)
Department of Physics
Jashore University of Science and Technology
Jashore 7408, Bangladesh

Part-time Faculty (January 2018 – December 2018)
Department of Theoretical Physics
University of Dhaka
Dhaka 1000, Bangladesh

Assistant Professor of Physics (November 2013 – November 2018)
Department of Arts and Sciences
Ahsanullah University of Science and Technology
Tejgaon, Dhaka 1208, Bangladesh

Teaching Assistant (February 2014 – October 2016)
School of Physics and Astronomy
University of Nottingham
Nottingham, United Kingdom

Lecturer in Physics (September 2010 – October 2013)
Department of Arts and Sciences
Ahsanullah University of Science and Technology
Tejgaon, Dhaka 1208, Bangladesh

RESEARCH GRANTS

Research Project 2024-2025 funded by Jashore University of Science and Technology
Funded amount: 550,000.00 BDT
Project title: Developing Efficient Lead-Free Double Perovskites: A First-Principle Path to Eco-Friendly Innovation

Research Project 2022-2023 funded by Jashore University of Science and Technology
Funded amount: 600,000.00 BDT
Project title: Making progress towards lead free efficient perovskite solar cells: A DFT study

Research Project 2021-2022 funded by University Grants Commission (UGC)
Funded amount: 300,000.00 BDT
Project title: Effect of radiation on the mechanical properties of shielding materials: A DFT study

EDUCATION

PhD in Physics (November 2013 – April 2017)
School of Physics and Astronomy
University of Nottingham
Nottingham, NG7 2RD, United Kingdom

Diploma in Condensed Matter Physics 2009 – 2010
The Abdus Salam International Center for Theoretical Physics (ICTP)
Strada Costiera 11, I-34151 Trieste, Italy

M. S. in Physics, 2005 (Exam held in 2008), 1st Class
Department of Physics, University of Dhaka
Dhaka 1000, Bangladesh

B. S. in Physics, 2004 (Exam held in 2006), 1st Class
Department of Physics, University of Dhaka
Dhaka 1000, Bangladesh

TITLE OF PhD THESIS

Theoretical Interpretation of Scanning Probe Images of Molecules on Surfaces

TITLE OF DIPLOMA THESIS

A Classical Potential for the Gold-Alkanethiols Interface

TITLE OF MASTER'S THESIS

Studies of Phonon Dispersion and Electronic Transport Properties of Amorphous Metals

LIST OF PUBLICATIONS

S. Zahan, O. Alsalmi, A.Z. Z. Ahmed, **Mohammad Abdur Rashid**, "Band gap modulation and improved optoelectronic and thermoelectric properties in Sn-doped $RbCaCl_3$ perovskites", **Physica B: Condensed Matter** 717, 417831 (2025), doi.org/10.1016/j.physb.2025.417831

S. Jaman, K. M. Kamruzzaman, M. R. Rokon, F. Farjana, **Mohammad Abdur Rashid**, M. B. Asfia "Comprehensive first-principles study of structural, electronic, optical, and elastic properties of $FrBCl_3$ (B = Mg & Ba) cubic perovskites", **Next Sustainability** 6, 100169 (2025), doi.org/10.1016/j.nxsust.2025.100169

S. Zahan, **Mohammad Abdur Rashid**, T. Afroze, M.H.R. Khan, "Comprehensive study of Sr2VInO6 and Sr2VTlO6: Structural, mechanical, optoelectronic and thermoelectric properties", **Materials Science and Engineering B** 317, 118223 (2025), doi.org/10.1016/j.mseb.2025.118223

S. Zahan, D. Afroj, **Mohammad Abdur Rashid**, "Impact of pressure on structural, mechanical, optoelectronic and thermoelectric properties of vacancy-ordered double perovskite K2SeCl6: A first principles study", **Next Materials** 8, 100512 (2025), doi.org/10.1016/j.nxmate.2025.100512

S. Jaman, R. C. Karmkar, **Mohammad Abdur Rashid,** M. B. Asfia, "Semiconductor to semimetallic transition in halide perovskite FrBCl3 (B = Ge, Sn) under hydrostatic pressure: A DFT insights", **Computational Condensed Matter** 42, e00995 (2025), doi.org/10.1016/j.cocom.2024.e00995

O. Alsalmia, **Mohammad Abdur Rashid**, "Study of structural, mechanical, thermal, and electronic structure properties of A2SnCl6 (A = Cs, Rb) perovskites for energy generation applications", **Journal of Ovonic Research** 20(4), 537 (2024), doi.org/10.15251/JOR.2024.204.537

A. M. Afridi, N. A. Nipa, **Mohammad Abdur Rashid**, "First-principle investigation of lead-free double perovskites Cs2MScCl6 (M = Na, K) for optoelectronic and thermoelectric applications", **Physica Scripta** 99, 055938 (2024), doi.org/10.1088/1402-4896/ad38e9

N. A. Nipa, A. M. Afridi, **Mohammad Abdur Rashid**, "Band gap and optical property modulation under pressure in vacancy-ordered double perovskite Cs_2SeCl_6", **Computational and Theoretical Chemistry** 1235, 114572 (2024), doi.org/10.1016/j.comptc.2024.114572

A. Raihan, **Mohammad Abdur Rashid**, M. H. Fahim, A. Hossain, M. R. Amin, "Investigation of lead-free direct bandgap Ca_2MAsO_6 (M = Ga, In) double perovskites for optoelectronic and thermoelectric applications: A first principles study", **Materials Science in Semiconductor Processing** 177, 108356 (2024), doi.org/10.1016/j.mssp.2024.108356

S. Jaman, M. B. Asfia, **Mohammad Abdur Rashid**, "Band gap engineering and enhanced optoelectronic performance by varying dopant concentration in $RbSr_{1-x}Sn_xCl_3$: Ab-inito study", **Physica B: Condensed Matter** 678, 415779 (2024), doi.org/10.1016/j.physb.2024.415779

Y. Naimi, A. Jafari, M. **Mohammad Abdur Rashid**, "Half-metallic Na-based half-Heusler alloys as potential spintronic materials", **Optical and Quantum Electronics** 56, 691 (2024), doi.org/10.1007/s11082-024-06307-9

M. H. Fahim, **Mohammad Abdur Rashid**, M. R. Amin, "A comprehensive DFT study of the optoelectronic, mechanical, and thermoelectric properties of $Rb_2NaScCl_6$ double perovskite implying different pressures", **Materials Today Communications** 38, 108093 (2024), doi.org/10.1016/j.mtcomm.2024.108093

M. Naseri, S. Amirian, M. Faraji, **Mohammad Abdur Rashid**, M. P. Lourenço, V. Thangadurai & D. R. Salahub, "Perovskenes: two-dimensional perovskite-type monolayer materials predicted by first-principles calculations", **Physical Chemistry Chemical Physics** 26, 946-957 (2024), dx.doi.org/10.1039/D3CP04435A

A. Allen, **Mohammad Abdur Rashid**, P. Rahe, S. P. Jarvis, J. N. O'Shea, J. L. Dunn & P. Moriarty, "Self-assembly and tiling of a prochiral hydrogen-bonded network: bi-isonicotinic acid on coinage metal surfaces", **Molecular Physics** 121:7-8, e2192824 (2023), doi.org/10.1080/00268976.2023.2192824

M. Naseri, D. R. Salahub, S. Amirian, H. Shahmohamadi, **Mohammad Abdur Rashid**, M. Faraji, N. Fatahi, "Multi-functional lead-free Ba_2XSbO_6 (X = Al, Ga) double perovskites with direct bandgaps for photocatalytic and thermoelectric applications: A first principles study", **Materials Today Communications** 35, 105617 (2023), doi.org/10.1016/j.mtcomm.2023.105617

M. B. Asfia and **Mohammad Abdur Rashid**, "First principles calculations of structural, electronic and optical properties of Sn-doped ZnS", **Physica B: Condensed Matter** 646, 414335 (2022), doi.org/10.1016/j.physb.2022.414335

M. B. Asfia, S. Jaman and **Mohammad Abdur Rashid**, "Pressure induced band gap shifting from ultra-violet to visible region of $RbSrCl_3$ perovskite", **Materials Research Express** 9, 095902 (2022), doi.org/10.1088/2053-1591/ac8f88

M. Naseri, D. R. Salahub, S. Amirian and **Mohammad Abdur Rashid**, "Computational investigation of Ba_2ZrTiO_6 double perovskite for optoelectronic and thermoelectric applications", **Journal of Solid State Chemistry** 314, 123385 (2022), doi.org/10.1016/j.jssc.2022.123385

Mohammad Abdur Rashid, M. Saiduzzaman, A. Biswas and K. M. Hossain, "First-principles calculations to explore the metallic behavior of semiconducting lead-free halide perovskites $RbSnX_3$ (X = Cl, Br) under pressure", **European Physical Journal Plus** 137, 649 (2022), doi.org/10.1140/epjp/s13360-022-02843-z

M. B. Asfia and **Mohammad Abdur Rashid**, "First-Principles Study of Half Metallic Ferromagnetic and Optical Properties of Nb Doped Cubic ZnS using TB-mBJ Approximation", **Dhaka University Journal of Science** 69(3), 194-201 (2022), doi.org/10.3329/dujs.v69i3.60030

W. A. Dujana, A. Podder, O. Das, Md. Solayman, M. T. Nasir, **Mohammad Abdur Rashid**, Md Saiduzzaman, and M. A. Hadi: "Structural, electronic, mechanical, thermal, and optical properties of UIr_3 under pressure: A comprehensive DFT study", **AIP Advances** 11, 105205 (2021), doi.org/10.1063/5.0064021

Md. Alamgir Badsha, Md. Humaun Kabir, **Mohammad Abdur Rashid**: "Coherent perfect absorption in unpatterned thin films of intrinsic semiconductor", **Journal of Optics** 49 (3) 342-350 (2020), doi.org/10.1007/s12596-020-00624-4

Md. Alamgir Badsha, **Mohammad Abdur Rashid**, Md. Humaun Kabir, Md. Mehade Hasan: "Coherent perfect absorption in epsilon-near-zero ITO thin film in near infrared", **Opt. Pura Apl.** 53(1), 1-12 (2020), doi.org/10.7149/OPA.53.1.51031

M. S. S. Chowdhury, **Mohammad A. Rashid**, M. A. Rahman and A. Z. Ziauddin Ahmed: "Study of Energy of Formation for Fe_xNi_{1-x} Liquid Binary Alloys", **Asian J. of Research and Reviews in Physics** 2(4), 1-12 (2019), doi.org/10.9734/ajr2p/2019/v2i430105

Adam Sweetman, **Mohammad A. Rashid,** Samuel P. Jarvis, Janette L. Dunn, Philipp Rahe and Philip Moriarty: "Visualizing the orientational dependence of an intermolecular potential", **Nature Communications** 7, 10621 (2016), doi.org/10.1038/ncomms10621

Adam Sweetman, Samuel P. Jarvis and **Mohammad A. Rashid:** "Modelling of 'sub-atomic' contrast resulting from back-bonding on Si(111)-7×7", **Beilstein Journal of Nanotechnology** 7, 937 (2016), doi.org/10.3762/bjnano.7.85

Samuel Paul Jarvis, **Mohammad Abdur Rashid,** Adam Sweetman, Jeremy Leaf, Simon Taylor, Philip Moriarty and Janette Dunn: "Intermolecular artifacts in probe microscope images of C_{60} assemblies", **Physical Review B** 92, 241405(R) (2015), doi.org/10.1103/PhysRevB.92.241405

M. Abdur Rashid and S. Scandolo: "A classical potential for the Gold (111)-Alkanethiols interface", **The AUST Journal of Science and Technology**, 4(1), 1 (2012)

PAPER IN INTERNATIONAL CONFERENCE

Md. Arafat Hosein, Salma Zahan, **Mohammad Abdur Rashid**: "Pressure dependent mechanical and optoelectronic properties of K_2TeCl_6 vacancy-ordered double perovskite: A DFT study", International Conference on Physics – 2024, Dhaka, Bangladesh, May 2024

Rupa Yasmin, **Mohammad Abdur Rashid**: "Exploring the effect of hydrostatic pressure on the optoelectronic and thermoelectric activities of potassium-based double perovskite K_2AgSbI_6", International Conference on Physics – 2024, Dhaka, Bangladesh, May 2024

Mst. Shahida Afrin, **Mohammad Abdur Rashid**: "Pressure dependent optoelectronic and thermoelectric characteristics of halide double perovskite K_2YAgBr_6 for energy storage applications: A first principles study", International Conference on Physics – 2024, Dhaka, Bangladesh, May 2024

Mohammad Abdur Rashid, A. Z. Z. Ahmed: "Pressure-Induced Tuning of Bandgap in Double Perovskite $Cs_2AgSbCl_6$: A Comprehensive DFT Study using TB-mBJ potential", 1st National Conference on Advances in Science and Technology (NCAST), BUET, Bangladesh (December 2023)

Mohammad Abdur Rashid, A. Z. Z. Ahmed: "Pressure-induced modulation of structural and optoelectronic properties in halide perovskite $CdYF_3$: A DFT study with TB-mBJ potential", 8th Conference of Bangladesh Crystallographic Association (BCA), DU, Bangladesh (November 2023)

Mohammad Abdur Rashid, Md. Borhanul Asfia, Sahadat Jaman: "Unveiling the impact of pressure on the opto-electronic and thermoelectric characteristics of $FrCaX_3$ (X = Cl, Br, I) perovskite materials: A first-principle investigation", International Conference on Physics for Sustainable Development and Technology (ICPSDT-2023), CUET, Bangladesh (September 2023)

Mohammad Abdur Rashid, Md. Borhanul Asfia, Sahadat Jaman: "Pressure induced opto-electronic, elasto-mechanical and thermoelectric properties of cubic $FrBCl_3$ (B = Ge, Sn): DFT investigation", International Conference on Electronics and Informatics 2022, Dhaka, Bangladesh (January 2023)

Mohammad Abdur Rashid, Md. Ohiduzzaman: "Electronic, magnetic, and optical properties of the Heusler compounds NbMn2(Si, Ge) using TB-mBJ potential", International Conference on Physics-2022, Dhaka, Bangladesh, May 2022

Salma Zahan, **Mohammad Abdur Rashid**: "Electronic and Optical properties of Nb doped rutile TiO_2: A DFT study", International Conference on Physics-2022, Dhaka, Bangladesh, May 2022

Kanij Fatima, Salma Zahan, Mst. Shahida Afrin, **Mohammad Abdur Rashid**: "Half-metallic behavior with high magnetic moment of half-Heusler alloys MCrPb (M = Hf, Zr): insights from DFT", International Conference on Physics-2022, Dhaka, Bangladesh, May 2022

Mst. Shahida Afrin, **Mohammad Abdur Rashid**: "Structural, electronic, magnetic and optical properties of full-Heusler alloy Zr2NiB", International Conference on Physics-2022, Dhaka, Bangladesh, May 2022

M. A. Rashid, P. Moriarty and J. L. Dunn: "Interpreting AFM images of the assembly of bi-isonicotinic acid molecules", International Conference on Physics-2020, Dhaka, Bangladesh, March 2020

M. A. Rashid, S. P. Jarvis, A. Sweetman, A. Saywell, P. Moriarty, J. L. Dunn: "Theoretical Study of The Intra- and Intermolecular Potentials of Assemblies of C_{60} Molecules and of Phthalocyanine Molecules", 19th International Conference on Non-Contact Atomic Force Microscopy, Nottingham, UK, July 2016

M. A. Rashid, S. P. Jarvis, A. Sweetman, P. Moriarty, J. L. Dunn: "Theoretical Study of the Intermolecular Potential (Artefact) Between C_{60} Molecules", UK-Japan Symposium on Atomic and Molecular Manipulation: Force and Tunnel Current in Scanning Probe Microscopy, Nottingham, UK, December 2015

M. A. Rashid, P. Sharp, P. Moriarty, J. L. Dunn: "Theoretical Study of $C_{60}F_{48}$ Using Hückel Molecular Orbital Theory", Interdisciplinary Surface Science Conference (ISSC-20), Birmingham, UK, March 2015

M. A. Rashid, S. Scandolo, S. K. Bhattacharya: "A Classical Potential for the Gold-Alkanethiols Interface", BPS Conference 2011, Dhaka, Bangladesh, February 2011

G. M. Bhuiyan, **M. A. Rashid**, A. Z. Ziauddin Ahmed and R. I. M. A. Rashid: "A Theory of Electrical Resistivity of Amorphous Metals", DPG Spring Meeting 2009, Dresden, Germany, March 2009

WORKSHOP ATTENDED

MSSC2024 - Ab initio Modelling in Solid State Chemistry, Department of Chemistry, South Kensington Campus, SW7 2AZ, London (online), 16-20 September 2024

WIEN2k Hands-On Workshop for New and Existing Users, The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, 08-19 April 2024

2D Materials for Spin-Orbitronics, The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy (online), 3-5 May 2024

CECAM Tutorial **Computational Spectroscopy Using Quantum Espresso and Related Codes**, SISSA, Trieste, Italy, 26-30 July 2010

Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics, SISSA, Trieste, Italy, 5-23 July 2010

Workshop on Dynamics of Strongly Correlated Quantum Systems, The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, 21-25 June 2010

Spring College on Computational Nanoscience, The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, 17-28 May 2010

Bose Winter School on Current Topics: Quantization, Wavelets and Their Applications to Physics-07, Department of Physics, University of Dhaka, Bangladesh & The Abdus Salam ICTP, Italy, December 2007

REFERENCES

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