# 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 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), 1<sup>st</sup> Class Department of Physics, University of Dhaka Dhaka 1000, Bangladesh

B. S. in Physics, 2004 (Exam held in 2006), 1<sup>st</sup> 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

M. H. Fahim, **Mohammad Abdur Rashid**, M. R. Amin, "A comprehensive DFT study of the optoelectronic, mechanical, and thermoelectric properties of Rb<sub>2</sub>NaScCl<sub>6</sub> double perovskite implying different pressures", **Materials Today Communications** 38, 108093 (2024), <u>doi.org/10.1016/j.mtcomm.2024.108093</u>

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), <u>dx.doi.org/10.1039/D3CP04435A</u>

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: biisonicotinic acid on coinage metal surfaces", **Molecular Physics** 121:7-8, e2192824 (2023), <u>doi.org/10.1080/00268976.2023.2192824</u>

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), <u>doi.org/10.1016/j.physb.2022.414335</u>

M. B. Asfia, S. Jaman and **Mohammad Abdur Rashid**, "Pressure induced band gap shifting from ultra-violet to visible region of RbSrCl<sub>3</sub> perovskite", **Materials Research Express** 9, 095902 (2022), <u>doi.org/10.1088/2053-1591/ac8f88</u>

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, "Firstprinciples 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), <u>doi.org/10.1140/epip/s13360-022-02843-z</u>

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<sub>3</sub> under pressure: A comprehensive DFT study", **AIP** Advances 11, 105205 (2021), <u>doi.org/10.1063/5.0064021</u>

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), <u>doi.org/10.7149/OPA.53.1.51031</u>

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), <u>doi.org/10.1038/ncomms10621</u>

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

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<sub>60</sub> 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)

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# PAPER IN INTERNATIONAL CONFERENCE

**Mohammad Abdur Rashid**, A. Z. Z. Ahmed: "Pressure-Induced Tuning of Bandgap in Double Perovskite Cs<sub>2</sub>AgSbCl<sub>6</sub>: A Comprehensive DFT Study using TB-mBJ potential", 1<sup>st</sup> 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<sub>3</sub>: A DFT study with TB-mBJ potential", 8<sup>th</sup> 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<sub>2</sub>: A DFT study", International Conference on Physics-2022, Dhaka, Bangladesh, May 2022

Kanij Fatima, Salma Zahan, Mst. Shahida Afrin, **Mohammad Abdur Rashid**: "Halfmetallic 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<sub>60</sub> 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<sub>60</sub>F<sub>48</sub> 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

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**, ICTP, Trieste, Italy, 21-25 June 2010

Spring College on Computational Nanoscience, 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

#### Dr. Janette Dunn

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#### **Prof. Philip Moriarty**

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