Md Imrul Reza Shishir

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Website • **Github** • **Google Scholar** • **Linkedin**

SUMMARY

- Ph.D. candidate in mechanical engineering with specialization in deep learning, machine learning, atomistic simulations (molecular dynamics (MD)), image segmentation, dislocations and grain boundaries, computational fracture mechanics, solid mechanics, finite element analysis (FEA), and topology optimization
- Experienced in high-performance computing (HPC) to simulate nanomaterials using molecular dynamics simulations and deep learning for computer vision problems in material science
- 5 years of working experience as a teaching assistant or instructor (tutorials, invigilation, and scrutiny) in UNC Charlotte and Inha University for different undergraduate courses i.e., Materials and Mechanics lab, Introduction of Solid Mechanics, and Introduction of Finite Element Method
- Good leadership and hands-on project management experience (4 years) in downstream oil and gas industries at various roles i.e., engineering design construction supervision, procurement, and commissioning
- Strong interpersonal communication skills, high adaptability, and collaborative team player mind-set

RESEARCH INTEREST

- Introducing a deep learning model to understand and design materials properties
- Implement a deep learning-based model to understand dislocations and grain boundaries in polycrystalline materials
- Molecular dynamics modeling to understand the behavior of materials and improve material properties
- Modeling fracture and damage in materials using the finite element method and atomistic simulations
- Topology optimization for different problems
- Developing linear and nonlinear finite element codes

EDUCATION

Doctor of Philosophy in Mechanical Engineering August 2022 (Anticipated)
The University of North Carolina at Charlotte, NC, USA. CGPA: 3.75/ 4.0
Dissertation project : **"Study of fracture properties of graphene-like two-dimensional material"**

Master of Engineering in Mechanical Engineering August 2017
Inha University, Incheon, Republic of Korea. CGPA: 4.19/ 4.5
Thesis project : **"Atomistic molecular dynamics simulation of cellulose microfibrils (CMF) and their interaction."**

Bachelor of Science in Mechanical Engineering March 2012
Bangladesh University of Engineering & Technology (BUET), Dhaka, Bangladesh. CGPA: 3.23/ 4.0
Thesis project : **"Experimental study and modeling low temperature organic rankine cycle."**

RESEARCH EXPERIENCE

University of North Carolina at Charlotte, Charlotte, NC January 2018 - Present
***Research Assistant**, Multiscale Material Modeling Laboratory*

- Introduced neural network model (physics informed neural network (PINN)) for topology optimization and size optimization to investigate the elastic and thermomechanical problems (python, JAX, ABAQUS)
- Implemented generative adversarial networks model to predict complete stress tensor for 2D polycrystalline materials using computer vision (Python, LAMMPS, OVITO)
- Developed deep learning models to predict fracture and grain properties for polycrystalline graphene using MD Simulations data (LAMMPS, OVITO, python) through computer vision
- Developed deep learning models to predict crack propagation paths and image segmentation model for polycrystalline graphene using MD Simulations data (LAMMPS, OVITO, python) through computer vision
- Assessed the failure criterion of polycrystalline graphene under biaxial loading using molecular dynamics simulations (LAMMPS, VMD, OVITO, Python)
- Extracted the traction–separation relations of symmetric grain boundaries of bi-crystalline graphene (LAMMPS, VMD, OVITO, Python)

- Investigated mechanical and fracture properties of 2D materials using molecular dynamics simulations (LAMMPS, VMD, MATLAB) to understand crack propagation and verified constitutive theory of fracture mechanics

Center for NCFC, **Inha University,** Incheon, KOR August 2015- August 2017
Research Assistant

- Measured mechanical and thermal properties of cellulose microfibrils (CMF) using atomistic simulation (GROMACS, VMD, MATLAB) and finite element method (FEM)
- Explored the application of chipless passive RFID sensor as a structural health-monitoring sensor by design, fabrication, and characterization of cross-type FSS array and HFSS simulations for FSS element (ANSYS HFSS)
- Analyzed the mechanical properties of cellulose nanocrystal/graphene oxide composite film and characterized as a humidity sensor.
- Synthesis of hydrogels and characterization for reconfigurable lens actuators
- Examined the ultrasonic wave propagation in piezoelectric polymer substrate to understand the tactile behavior both computationally and experimentally

TEACHING EXPERIENCE

University of North Carolina at Charlotte, Charlotte, NC January 2018 - May 2021
***Teaching Assistant**, Mechanics & Materials Lab (MEGR 3152 Mechanics & Materials Lab)*

- Designed and conducted laboratory session for undergraduate classes
- Short lecture about the technical background of the experiment.
- Trained over 180 students for hands-on experience for various mechanical testing and measurements i.e., tensile strength testing, hardness testing, impact toughness, heat treatment, metallography, SEM, fatigue for metals or polymers

University of North Carolina at Charlotte, Charlotte, NC May 2018- August 2018
***Teaching Assistant**, MEGR 2144 Introduction to Solid Mechanics*

- Designed the homework and graded the homework, midterm exam and final exam
- Mentored over 30 students for the course materials and example solving

Inha University, Incheon, KOR August 2015- December 2015
***Teaching Assistant**, Introduction to Finite Element Method*

- Graded the homework, midterm exam and final exam of undergraduate course
- Guided over 30 students for hands-on training on finite element software

PUBLICATIONS (https://scholar.google.co.kr/citations?user=aHz1SeoAAAAJ&hl=en)

Journal Article ("*"as a 1st Author)

- **Shishir, MD Imrul Reza,** and Alireza Tabarraei. *"Topology optimization through machine learning."* **(In manuscript preparation)** *
- **Shishir, MD Imrul Reza,** and Alireza Tabarraei. *"Deep learning model to predict the complete stress tensors of polycrystalline graphene."* **(In manuscript preparation)** *
- **Shishir, MD Imrul Reza,** and Alireza Tabarraei. *"Atomistic molecular dynamics simulation based failure criterion of polycrystalline graphene under biaxial loading."* **(In manuscript preparation)** *
- **Shishir, MD Imrul Reza,** Mohan Surya Raja Elapolu, and Alireza Tabarraei. *"Data driven deep learning model to predict the mechanical properties of polycrystalline graphene."* **(In submission)** *
- Elapolu, Mohan SR, **Md Imrul Reza Shishir**, and Alireza Tabarraei. *"A novel approach for studying crack propagation in polycrystalline graphene using machine learning algorithms."* Computational Materials Science 201 (2022): 110878. DOI: https://doi.org/10.1016/j.commatsci.2021.110878
- **Shishir, MD Imrul Reza,** Mohan Surya Raja Elapolu, and Alireza Tabarraei. *"Investigation of fracture and mechanical properties of monolayer C3N using molecular dynamic simulations."* Mechanics of Materials 160 (2021): 103895. DOI: https://doi.org/10.1016/j.mechmat.2021.103895 *

- **Shishir, MD Imrul Reza,** and Alireza Tabarraei. *"Traction-separation laws of graphene grain boundaries."* Physical Chemistry Chemical Physics 23, no. 26 (2021): 14284-14295. DOI: https://doi.org/10.1039/D1CP01569A *

- **Shishir, MD Imrul Reza,** Abdullahil Kafy, and Jaehwan Kim. *"An investigation of the thermal response of the crystalline structure in cellulose Iβ by atomistic molecular dynamic simulation"* **(In submission)** *

- **Shishir, MD Imdul Reza,** Seongcheol Mun, Hyun-Chan Kim, Jeong Woong Kim, and Jaehwan Kim. *"Frequency-selective surface-based chipless passive RFID sensor for detecting damage location."* Structural Control and Health Monitoring 27, no. 3 (2020): e2511. DOI: https://doi.org/10.1002/stc.2511 *

- Akther, Asma, Abdullahil Kafy, Lindong Zhai, Hyun Chan Kim, **MD Imrul Reza Shishir**, and Jaehwan Kim. *"Ultrasonic wave propagation of flexible piezoelectric polymer for tactile actuator: simulation and experiment."* Smart Materials and Structures 25, no. 11 (2016): 115043. DOI: https://doi.org/10.1088/0964-1726/25/11/115043

- Jayaramudu, Tippabattini, Yaguang Li, Hyun-U. Ko, **Imrul Reza Shishir**, and Jaehwan Kim. *"Poly (acrylic acid)-Poly (vinyl alcohol) hydrogels for reconfigurable lens actuators."* International Journal of Precision Engineering and Manufacturing-Green Technology 3, no. 4 (2016): 375-379. DOI: https://doi.org/10.1007/s40684-016-0047-x

- Kafy, Abdullahil, Asma Akther, **Md Imrul Reza Shishir**, Hyun Chan Kim, Youngmin Yun, and Jaehwan Kim. *"Cellulose nanocrystal/graphene oxide composite film as humidity sensor."* Sensors and Actuators A: Physical 247 (2016): 221-226. DOI: https://doi.org/10.1016/j.sna.2016.05.045

Conference Paper ("*"as a 1st Author)

- **Shishir, MD Imrul Reza**, Mohan Surya Raja Elapolu, and Alireza Tabarraei. *"A Deep Convolutional Neural Network-Based Method to Predict Accurate Fracture Strength of Poly-Crystalline Graphene."* In ASME International Mechanical Engineering Congress and Exposition, vol. 85680, p. V012T12A012. American Society of Mechanical Engineers, 2021. https://doi.org/10.1115/IMECE2021-70580 *

- **Shishir, MD Imrul Reza**, and Alireza Tabarraei. *"Atomistic molecular dynamics simulation based failure criterion of polycrystalline graphene under biaxial loading."* In ASME International Mechanical Engineering Congress and Exposition, vol. 84607, p. V012T12A035. American Society of Mechanical Engineers, 2020. DOI: https://doi.org/10.1115/IMECE2020-24567 *

- **Shishir, MD Imrul Reza**, and Alireza Tabarraei. *"Molecular Dynamics Simulation Based Cohesive Zone Representation of Intergranular Fracture Processes in Bicrystalline Graphene."* In ASME International Mechanical Engineering Congress and Exposition, vol. 84607, p. V012T12A028. American Society of Mechanical Engineers, 2020. DOI: https://doi.org/10.1115/IMECE2020-23624 *

- **Shishir, MD Imrul Reza**, and Alireza Tabarraei. "A molecular dynamic study of nano-fracture of C_3N." In ASME International Mechanical Engineering Congress and Exposition, vol. 59469, p. V009T11A051. American Society of Mechanical Engineers, 2019. DOI: https://doi.org/10.1115/IMECE2019-11543 *

- Muthoka, Ruth M., **MD Imrul Reza Shishir**, Hyun Chan Kim, Jung Woong Kim, and Jaehwan Kim. *"Atomistic molecular dynamics study to investigate thermal response of cellulose nanofibrils using GROMACS."* In Nano-, Bio-, Info-Tech Sensors, and 3D Systems II, vol. 10597, p. 105971F. International Society for Optics and Photonics, 2018. DOI: https://doi.org/10.1117/12.2296841

- **Shishir, Md Imrul Reza**, Hyun Chan Kim, Lindong Zhai, Abdullahil Kafy, Jung Woong Kim, Mwongeli Ruth, Jaehwan Kim, *"Atomistic Molecular Dynamics investigation of Cellulose Nanofibril structure".* The 4th International Cellulose Conference, Fukuoka, Japan 2017. *****

- Kafy, Abdullahil, Asma Akther, **MD IR Shishir,** and Jaehwan Kim. *"Cellulose/graphene oxide composite for electrode materials of flexible energy devices."* In Nanosensors, Biosensors, Info-Tech Sensors and 3D Systems 2017, vol. 10167, p. 101670Q. International Society for Optics and Photonics, 2017. DOI: https://doi.org/10.1117/12.2259838

- Kafy, Abdullahil, Asma Akther, **Md IR Shishir,** Eun Byul Jo, and Jaehwan Kim. *"Synthesis and characterization of cellulose nanocrystal/graphene oxide blended films."* In Nanosensors, Biosensors, and Info-Tech Sensors and

Systems 2016, vol. 9802, p. 980204. International Society for Optics and Photonics, 2016. DOI: https://doi.org/10.1117/12.2219656

- Sanjid, A., H. H. Masjuki, M. A. Kalam, SM Ashrafur Rahman, M. J. Abedin, **M. I. Reza**, and H. Sajjad. *"Experimental investigation of palm-jatropha combined blend properties, performance, exhaust emission and noise in an unmodified diesel engine."* Procedia Engineering 90 (2014): 397-402. DOI: https://doi.org/10.1016/j.proeng.2014.11.868

- Azad, Abul Kalam, M. G. Rasul, Rubayat Islam, and **Imrul Reza Shishir**. *"Analysis of wind energy prospect for power generation by three Weibull distribution methods."* Energy Procedia 75 (2015): 722-727. DOI: https://doi.org/10.1016/j.egypro.2015.07.499

Poster ("*"as a 1st Author)

- **Shishir, MD Imrul Reza**, Alireza Tabarraei, *"A molecular dynamic study of nano-fracture of C_3N"* The ASME 2019 International Mechanical Engineering Congress and Exposition, Salt Lake City, Utah, USA, 2019. *

- **Shishir, MD Imrul Reza**,Ruth Mwongeli Muthoka, Jung Woong Kim, and Jaehwan Kim zJung Woong Kim, and Jaehwan Kim, *"Investigation into the role of hydrogen bond in cellulose nanofibril by atomistic molecular dynamics."* Korean Society of Presicion Engineer Spring Conference, Jeju, Republic of Korea, 2017. *

- **Shishir, Imrul Reza,** Abul Kalam Azad, and Tanjim Ahmed. *"Electricity Generation Based On Biomass Residue: Scope, Relevance And Applications."* Sixth BSME-LCTE 2014 (2014): 1-7. *

PRESENTATION

- Technical presentation " A Deep Convolutional Neural Network-Based Method to Predict Accurate Fracture Strength of Poly-Crystalline Graphene." ASME, International Mechanical Engineering Congress and Exposition, November 2021 (IMECE2021)
- Technical presentation "Predict Fracture Stress of Poly-Crystalline Graphene Using Deep Learning." 16th U.S. National Congress on Computational Mechanics (Virtual), USACM, July 2021
- Technical presentation "Atomistic molecular dynamics simulation based failure criterion of polycrystalline graphene under biaxial loading." ASME, International Mechanical Engineering Congress and Exposition, November 2020 (IMECE2020)
- Technical presentation "Molecular Dynamics Simulation Based Cohesive Zone Representation of Intergranular Fracture Processes in Bicrystalline Graphene." ASME, International Mechanical Engineering Congress and Exposition, November 2020 (IMECE2020)
- Technical presentation "A molecular dynamic study of nano-fracture of C_3N." ASME, International Mechanical Engineering Congress and Exposition, November 2019 (IMECE2019)
- Academic presentation "A Molecular Dynamic Study of fracture properties of graphene." MEES graduate seminar series, UNC Charlotte, September 2019
- Onsite training presentation on "Basic Training on Codeware COMPRESS" and "Basic Training on Plant Design & 3D Modeling of Plant" 1250 BPD Condensate Fractionation Plant, Sylhet Gas Field Limited at Rashidpur, Bahubal, Habiganj, April 2013

GRANT WRITING WORKSHOP

- **"National Science Foundation (NSF): CISE Grant Writing Workshop"** arrange by the University of Louisiana at Lafayette (November 2021)
- **"National Institutes of Health (NIH) Grant Writing Workshop"** arrange by the University of Louisiana at Lafayette (October 2021)
- **"National Science Foundation (NSF): CBET CAREER Grant Writing Workshop"** arrange by the University of Louisiana at Lafayette (February 2021)

ACADEMIC WORKSHOP

- Short Course on **"Mechanistic Data Science for STEM Education and Applications"** Under USACM at 16th USNCCM congress, July 2021

- Workshop on **"spring seminar for computational chemistry2016@CSc"** Molecular dynamics and other computational chemistry technique was discussed and hands on training. **PRACE-CSC**, Espo, Finland, March 2016
- Short Course on **"Noise Control & Fire Fighting"** Under BUET-SIDA Project at BUET, Bangladesh. October 2011

HONORS

- **USNCCM16 Conference Award,** USACM, July 2021
- **Graduate School Summer Fellowship (GSSF),** UNC Charlotte, (Summer 2021)
- **GPSG Travel Grant,** UNC Charlotte, (Fall 2019, Fall 2020, Summer 2021)
- **President Award,** IoT Data Hackathon, Asian Data Week, November 2017
- **Best Graduate Researcher Award,** Inha University, August 2018.
- **Jungseok International Fellowship** (Inha University), (2015-2017)
- **Technical Scholarship** (BUET), From (2007-2011)
- **Board of Intermediate and Secondary Education Scholarship,** From (2004-2006)

EDUCATION COMPETITION

- Asian Data Week (2017) KISTI Urban IoT Data Hackathon: **Real-Time Human Tracking System.** (**President Award**)

PEER REVIEW

- Two manuscripts for IOPscience Nanotechnology peer reviewed journal
- Five manuscripts for IMECE-ASME peer reviewed conferenced

CONFERENCE VOLUNTEER

- **Session Chair,** Technical Session: 12-21-02: Data-Enabled Predictive Modeling, Machine Learning, and Uncertainty Quantification in Computational Mechanics, The ASME 2021 International Mechanical Engineering Congress and Exposition, Virtual, 2021.
- **Session Chair,** Technical Session: 11-12-2 Atomistic Scale Crack Nucleation and Propagation Modeling, The ASME 2019 International Mechanical Engineering Congress and Exposition, Salt Lake City, Utah, USA, 2019.
- **Conference Technical Session Coordinator,** assist the technicians and session chairs during the virtual four technical presentation sessions.

LEADERSHIP EXPERIENCE

Member, International Student Advisory Committee, UNC Charlotte	:	Fall 2021
Mentor, Exchange Student Mentor Program, UNC Charlotte	:	Fall 2021
Secretary, American Society for Computational Mechanics, UNC Charlotte	:	Spring 2021
President, Ekush-Bangladesh Student Organization, UNC Charlotte	:	October 2019 ~ October 2020
Senator, Graduate & Professional Student Government, UNC Charlotte	:	August 2018 ~ October 2019
Executive member, Ekush-Bangladesh Student Organization, UNC Charlotte	:	February 2018 ~ October 2019
Vice-Chairman, Greater Khulna Association of BUET Student, BUET	:	August 2009 ~ August 2010
Member, Association of Mechanical Engineer, BUET		June 2007 ~ March 2012

SKILLS

Software Skills :

- **Programming Language** (Python, MATLAB, Pearl, C++, Mathematica, Visual Basic, TCL)
- **Machine Learning and Image processing** (TensorFlow, Pytorch, Keras, sklearn, JAX, Elegy, OpenCV)
- **HPC Computing** (WinSCP, Putty, Slurm, Torque, Filezilla)
- **Molecular Dynamics** (LAMMPS, GROMACS)
- **Visualization** (VMD, OVITO)
- **Material Editor** (Material Studio, Avgrado)

- **CAM/CAD** (SOLIDWORKS, AutoCAD Inventor, AutoCAD Plant 3D, CADWorx)
- **Multiphysics Simulations** (ABAQUS, ANSYS, COMPRESS, COMSOL)

Laboratory Skills :
- Tensile or compression test (Universal testing machine) for metal and polymer
- Charpy impact test for metal
- Fatigue test for metal
- Metallography and heat treatment of metal
- Sample preparation and operation of scanning electron microscope and atomic force microscope

Communication Skill : Collaboration, Teamwork, Conference presentation, Article and technical report writing

Others : Git, LaTeX, Microsoft Word and Power Point, Excel, Unix Shell Scripting

PROFESSIONAL MEMBERSHIP

- **Member**, American Society of Mechanical Engineer **(ASME),** October, 2012-2013, October 2019~Present (Membership No: 100565143)
- **Member**, American Society of Civil Engineers **(ASCE)**
- **Member**, Korean Society of Precision Engineer **(KSPE)**
- **Member**, Society of Photographic Instrumentation Engineers **(ASCE)**
- **Member**, Institute of Engineers, Bangladesh

WORK EXPERIENCE

ZICOM Equipment Pte Ltd, Dhaka, Bangladesh January 2014-August 2015
Engineer *(Mechanical, Plant Design)*
- Supervised, designed, installed, and commissioned new equipment and fittings to ensure ongoing industry advantage for an EPC (Engineering, procurement, and construction) contractor in a downstream oil and gas process plant
- Designed pressure vessel & performed mechanical stress analysis & equipment sizing calculations by following the latest standards and industrial practices (ASME BPVC) (COMPRESS, AutoCAD Plant 3D, CADWorx)
- Designed pipe routing in 3D plant software with stress calculation to choose the right fittings for plant construction
- Prepared 3D Model & General Arrangement Diagram of Equipment
- Commissioned and report the non-destructive test of the weld joint for the pipe routing segment
- HAZOP study, HAZID study & Risk Assessment of the Plant

ZICOM Equipment Pte Ltd, Dhaka, Bangladesh June 2012-December 2013
Assistant Engineer *(Mechanical, Plant Design)*
- Designed, installed, and commissioned new equipment and fittings to ensure ongoing industry advantage for an EPC (Engineering, procurement, and construction) contractor in a downstream oil and gas process plant
- Designed pressure vessel & performed mechanical stress analysis & equipment sizing calculations by following the latest standards and industrial practices (ASME BPVC) (COMPRESS, AutoCAD Plant 3D, CADWorx)
- Designed pipe routing in 3D plant software with stress calculation to choose the right fittings for plant construction
- Prepared 3D Model & General Arrangement Diagram of Equipment
- Commissioned and report the non-destructive test of the weld joint for the pipe routing segment

INTERNSHIP

SUMMIT Power Limited, Comilla, Bangladesh August 2011 ~ September 2011
Intern (Mechanical Engineering)
- Observed the major schedule (10000 hours) maintenance of 100MW internal combustion engine powerplant.
- Documented the log report for the final report of the scheduled maintenance

INDUSTRIAL TRAINING

- **Training,** "(HAZOP) Hazard & Operability Method" by GT-Consultancy, Singapore : November 2012
- **Training,** "Mallard Ball Valve" by Circor Mallard Control, Singapore : November 2012

SOCIAL WORK/ EXTRACARICULAM ACTIVITIES

- **Associate Editor:** Agami Carolina Newsletter Team
- **Advisor for Editorial committee:** EKUSH-BSO UNC Charlotte Annual Newsletter
- **Volunteer**, NCEES Engineer week 'random acts of engineering (2018), Charlotte
- **Donor**, Quantum Foundation, Bangladesh (A Voluntary Blood Donor's Organization)
- **Donor**, BADHON blood donation organization (A Voluntary Blood Donor's Organization)
- **Member** of Runner-up RAG, 2011 Soccer Team
- **Member** of Dr. M. A. Rashid Hall Soccer Team, Inter- Hall Soccer Tournament
- **Member,** Debating Club, BUET

REFERENCES

1. **Dr. Alireza Tabarraei**
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   The University of North Carolina at Charlotte
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   Website: https://coefs.uncc.edu/atabarra/
   Relation: Dissertation Supervisor, Instructor for TA course (Introduction of Solid Mechanics)
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   Website: http://coefs.uncc.edu/hcheruku
   Relation: Dissertation committee member, Course Instructor
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3. **Dr. Terry T. Xu**
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   The University of North Carolina at Charlotte
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   Relation: Instructor for TA Course (Mechanics of Materials), Graduate advisor
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