

# Md Khayrul Islam

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## EDUCATION

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### Lehigh University

Pennsylvania, USA

*Ph.D. in Mechanical Engineering and Mechanics; GPA: 3.81/4.00*

*Jan 2021 – Current*

### Lehigh University

Pennsylvania, USA

*M.S. in Mechanical Engineering and Mechanics; GPA: 3.81/4.00*

*Jan 2021 – May 2023*

**Thesis Title:** Predicting Drug Loading in Extracellular Vesicles through Coarse-Grained Molecular Dynamics Simulation.

### Bangladesh University Engineering and Technology

Dhaka, Bangladesh

*B.Sc. in Industrial and Production Engineering; GPA: 3.55/4.00*

*Jun 2014 – Oct 2018*

**Thesis Title:** Molecular dynamics simulation of the mechanical properties of CNT-polyoxymethylene composite with a reactive forcefield.

## RESEARCH EXPERIENCE

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### Bio Nano Interface Lab

Lehigh University, Pennsylvania

*Graduate Research Assistant*

*Jan 2021 – Present*

- The study used coarse-grained molecular simulation to investigate the drug loading process in extracellular vesicles, focusing on the squeezing of vesicles to facilitate drug encapsulation and gaining insights into the underlying physical mechanisms.

**Impact:** The research analyzed the physical mechanisms involved in nanopore formation and cargo loading, offering valuable insights to guide nanofluidic device design for optimal drug loading. **NIH** Grant R01HL131750, R21EB033102 **NSF** CBET2039310

- A microfluidic vessel-on-a-chip platform was developed to study the key steps of tumor cell metastasis in blood vessels.

**Impact:** This study found specific biomechanical factors, like vascular surface properties and hemodynamic disturbances, can increase circulating tumor cell (CTC) adhesion. The computational models developed in the study could aid in understanding tumor metastasis progression and inspire new anticancer therapy ideas.

- A system using cell-laden beads assembled into an on-chip vessel network was developed to mimic tumor-tumor microenvironment interactions.

**Impact:** The system has the potential to improve preclinical drug discovery processes by enabling the large-scale fabrication of biomimetic in vitro tumor models.

- The study uses modeling and analysis to understand the factors that contribute to droplet resuspension and proposes strategies for minimizing the risk of infection during the COVID-19 pandemic.

**Impact:** The study sheds light on the transmission mechanism of COVID-19. The insights gained from the study may be useful in guiding public health guidelines and policies to minimize the risk of infection. **NSF** Grant 2039310

- Utilized deep learning to differentiate hematopoietic stem cells (HSCs) and multipotent progenitors (MPPs) based on their light microscopy images.

**Impact:** It offers a novel and efficient approach to differentiate HSCs and MPPs using deep learning based on cell morphology to accelerate stem cell research and improve the development of new stem cell therapies. **NSF** Grant EECS2215789

### Multiscale Mechanical Modeling and Research Network (MMMRN)

Dhaka, Bangladesh

*Undergraduate Research Assistant*

*Oct 2018 – Jan 2021*

- Molecular dynamics simulations were performed using a reactive force field (ReaxFF) to determine the changes in mechanical properties, and the study found that the use of SWCNT in the polymer matrix of POM significantly improves the resulting mechanical property.

**Impact:** The study shows the potential of using SWCNTs as additives to enhance the mechanical properties of POM composites. This finding may inform the development of new materials with improved properties and could have applications in various industries.

## WORK EXPERIENCE

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### Lehigh University

Bethlehem, Pennsylvania

*Teaching Assistant*

*Fall 2021 and Fall 2022*

- Instructor for the course of Heat and Mass Transfer

### GMS Composite Knitting Ind. Ltd.

Dhaka, Bangladesh

*Management Trainee*

*Feb 2018 – Aug 2018*

- Worked as a planning member and developed Excel VBA based automatic line balancing algorithm to balance swing line.
- Developed Floor based efficiency optimization system using Excel VBA to maximize overall floor efficiency with respect to the minimum machine which helps to increase around 8-12% efficiency of the swing floor.

### Panjeree Publication Ltd.

Dhaka, Bangladesh

*Writer*

*Dec 2015 – Dec 2017*

- Written complimentary book for the secondary and high secondary study of Bangladesh

## AWARDS & ACHIEVEMENTS

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- P.C. Rossin College of Engineering fellowship at Lehigh University
- SCEA- PTAK prize global case study competition scholarship
- Acknowledgement certificate for donating blood eight times during undergraduate studies
- Government Scholarship for outstanding result in Secondary school in Bangladesh

## SKILLS

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**Programming:** C, C++, Python, MATLAB, LAMMPS, Excel VBA

**Computer-Aided Design Tools:** AutoCAD, SolidWorks, Catia.

**Simulation software:** Materials Studio, AtomViewer, AtomEye, Proteus, Visual Molecular Dynamics (VMD), Ovito, COMSOL Multiphysics, ANSYS Fluent

## MEMBERSHIP

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- Blood donor at American red cross
- Graduate Student Association of Lehigh University

## PUBLICATIONS

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1. **Islam, Khayrul**, M Razizadeh, and Y Liu. Coarse-Grained molecular simulation of extracellular vesicles squeezing for drug loading. *Phys. Chem. Chem. Phys.*, 2023
2. Yue Wu, Yuwen Zhao, Yuyuan Zhou, **Islam, Khayrul**, and Yaling Liu. Microfluidic Droplet-Assisted fabrication of Vessel-Supported tumors for preclinical drug discovery. *ACS Appl. Mater. Interfaces*, 15(12):15152–15161, March 2023
3. Shen Wang, Jianzhong Han, Jingru Huang, Yuheng Shi, Yuyuan Zhou, Dongwook Kim, **Islam, Khayrul**, Jane Zhou, Olga Ostrovsky, Zhaorui Lian, Yaling Liu, and Jian Huang. Deep learning-based predictive identification of functional subpopulations of hematopoietic stem cells and multipotent progenitors. December 2022
4. Ratul Paul, Yuwen Zhao, Declan Coster, Xiaochen Qin, **Islam, Khayrul**, Yue Wu, and Yaling Liu. Rapid prototyping of high-resolution large format microfluidic device through maskless image guided in-situ photopolymerization. 2022
5. Yue Wu, Yuyuan Zhou, Ratul Paul, Xiaochen Qin, **Islam, Khayrul**, and Yaling Liu. Adaptable microfluidic Vessel-on-a-Chip platform for investigating tumor metastatic transport in bloodstream. *Anal. Chem.*, 94(35):12159–12166, September 2022

6. M Nikfar, R Paul, **Islam, Khayrul**, M Razizadeh, and others. Respiratory droplet resuspension near surfaces: Modeling and analysis. *Journal of Applied*, 2021
7. **Islam, Khayrul**, S Saha, and A K M Masud. Molecular dynamics simulation of the mechanical properties of CNT-polyoxymethylene composite with a reactive forcefield. *Mol. Simul.*, 2020

#### CONFERENCE PRESENTATIONS

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1. **Islam, Khayrul**, Yuwen Zhao, Shen Wang, and Yaling Liu. Machine learning based classification of cells by mechanical properties in microfluidic device. *48th Annual Northeast Bioengineering Conference (NEBEC 2022) (April 2022), Columbia University, New York City, New York*, 2022
2. **Islam, Khayrul**, Tahreen Nabila, and AKM. Masud. Investigation of the mechanical properties of polypropylene /carbon nanotube composite by molecular dynamics simulation. *13th International Conference on Mechanical Engineering, Dhaka, Bangladesh*, 2019