# Mohammad Babar

Website Google Scholar LinkedIn

**EDUCATION** 

Carnegie Mellon University

Pittsburgh, PA

Aug 2019 - Present

Email: mbabar@andrew.cmu.edu

Mobile: +1-412-320-1045

PhD in Mechanical Engineering; GPA: 4.0/4.0 Courses: Energy Storage and Systems, Advanced Thermodynamics, Molecular Simulation of Materials, Numerical Methods, Machine Learning for Mech. Eng. and AI, Bayesian Machine Learning, Intro. to Quantum Mechanics, Solid State Physics

Teaching Experience: Undergraduate Fluid Mechanics (2 semesters), Linear Algebra and Differential equations (2 semesters)

Carnegie Mellon University

Pittsburgh, PA

MS in Mechanical Engineering; GPA: 4.0/4.0

Aug 2019 - Dec 2022

Indian Institute of Technology

Delhi, India

Bachelor of Mechanical Engineering; GPA: 9.24/10.0

Aug 2015 - May 2019

# SKILLS SUMMARY

• Languages: Python, Julia

• Tools: Quantum Espresso, GPAW, Gaussian 09, FEniCS, Matlab, Mathematica, Adobe Illustrator

#### Publications

1. Effect of disorder and doping on electronic structure and diffusion properties of Li<sub>3</sub>V<sub>2</sub>O<sub>5</sub> M Babar, H Hafiz, Z Ahmad, B Barbiellini, A Bansil, V Viswanathan Journal of Physical Chemistry C 2022, 126, 37, 15549–15557

2. Tunable angle-dependent electrochemistry at twisted bilayer graphene with moiré flat bands Y Yu, K Zhang, H Parks, M Babar et al.

Nature Chemistry 14 (3), 267-273

3. An accurate machine learning calculator for the lithium-graphite system

M Babar, HL Parks, G Houchins, V Viswanathan

Journal of Physics: Energy 3 (1), 014005

4. Effect of surface conduction-induced electromigration on CMM for electroosmotic flow measurement

M Babar, K Dubey, SS Bahga

Electrophoresis 41 (7-8), 570-577

5. Nonlinear concentration waves in current monitoring method for measurement of electroosmotic flow (talk)

M Babar, K Dubey, S Singh Bahga

APS Division of Fluid Dynamics Meeting Abstracts, G36. 006

### Current Projects

#### 1. Twisto-electrochemistry in trilayer graphene system

Using Marcus Hush Chidsey theory with density of states and quantum capacitance to identify rate enhancement region around magic angle twisted trilayer graphene. Manuscript in preparation.

# 2. Machine learning steady state voltammograms for Gerischer model

Incorporating Gerischer model in obtaining steady state voltammograms for electrochemical reactions. Solving coupled Poisson and Nernst Planck equations in FEniCS PDE solver and generating input data for training a physics-informed neural network in flat band superconductors like twisted graphene systems.

#### 3. Predicting anionic redox in lithium rich transition metal cathodes

Studying Li-rich binary system for capacity increase through anionic redox by substituting transition metals in optimal concentration ratios using first principles modelling. Downselecting best candidates and characterizing redox orbitals using Compton scattering spectroscopy via collaborators in Japan.

# Honors and Awards

Selected to attend APS GERA energy workshop with reimbursement

March 2023

Won best poster award at Pittsburgh Quantum Institute conference Won conference travel award from Pittsburgh Quantum Institute

September 2022 May 2022

Selected to attend Topological Matter School 2021

August 2021

Won best poster award CMU MechE symposium

March 2021

Ranked in top five among 75 students in Undergraduate Mechanical Engineering branch

August 2019

Won Merit Award for three consecutive undergraduate semesters

May 2019