

# Mohammad Babar

Website Google Scholar LinkedIn

## EDUCATION

---

- **University of Michigan** Ann Arbor, MI  
*PhD in Mechanical Engineering* Present  
Thesis proposal: Atomic and Geometric Modifications for High Performance Lithium Ion Electrodes  
Advisor: Dr. Venkat Viswanathan, Committee: Dr. Efthimos Kaxiras (Harvard Physics), Dr. Vikram Gavini, Dr. Robert Hovden
- **Carnegie Mellon University** Pittsburgh, PA  
*MS in Mechanical Engineering; GPA: 4.0/4.0* Aug 2019 - Dec 2022  
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 Assistantship: Undergraduate Fluid Mechanics (2 semesters)
- **Indian Institute of Technology** Delhi, India  
*Bachelor of Mechanical Engineering; GPA: 9.25/10.0* Aug 2015 - May 2019  
Teaching Assistantship: Linear Algebra and Differential equations (2 semesters)

## SKILLS SUMMARY

---

- **Languages:** Python, Bash, Julia
- **Tools:** MATLAB, Quantum Espresso, Pytorch, FEniCS, COMSOL, PyBaMM, GPAW, LAMMPS, Gaussian, Mathematica, Git
- **Keywords:** Ab Initio · Monte Carlo · Physics-based Simulations · Electronic Structure · Design of Experiments · Battery modeling · Bayesian Optimization · Density Functional Theory · Machine learning Interatomic Potentials · Molecular Dynamics · Reaction Kinetics · Parameter Estimation · Computational Materials Science · Computational Chemistry · Electrochemistry · Finite Element Analysis · Thermodynamics · Fluid Mechanics · Li-ion Battery Chemistry · Solid State Physics

## PUBLICATIONS

---

1. Modeling Scanning Electrochemical Cell Microscopy (SECCM) in Twisted Bilayer Graphene  
**M Babar**, V Viswanathan  
Journal of Physical Chemistry Letters 2024
2. Twisto-electrochemical activity volcanoes in trilayer graphene  
**M Babar**, Z Zhu, R Kurchin, E Kaxiras, V Viswanathan  
Journal of the American Chemical Society 2024
3. Determining effects of doping lithium nickel oxide with tungsten using compton scattering  
V N Kothalawala, ..., **M Babar**, V Viswanathan, H Hafiz, A Bansil  
APL Energy 2 (2) 2024
4. Anomalous interfacial electron-transfer kinetics in twisted trilayer graphene caused by layer-specific localization  
K Zhang, Y Yu, S Carr, **M Babar** et al.  
ACS Central Science 9 (6), 1119-1128 2023
5. Effect of disorder and doping on electronic structure and diffusion properties of  $\text{Li}_3\text{V}_2\text{O}_5$   
**M Babar**, H Hafiz, Z Ahmad, B Barbiellini, A Bansil, V Viswanathan  
Journal of Physical Chemistry C, 126, 37, 15549–15557 2022
6. 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 2022
7. An accurate machine learning calculator for the lithium-graphite system  
**M Babar**, H L Parks, G Houchins, V Viswanathan  
Journal of Physics: Energy 3 (1), 014005 2020
8. Effect of surface conduction-induced electromigration on CMM for electroosmotic flow measurement  
**M Babar**, K Dubey, S S Bahga  
Electrophoresis 41 (7-8), 570-577 2020

## CURRENT PROJECTS

---

1. **Machine Learning-assisted Magnetic Moment Analysis in Lithium-rich Transition Metal Oxides**  
Classifying regions of anionic and cationic redox over the charge cycle using total and projected magnetic moment over species. Employing E(3) equivariant graph neural networks and universal ML potential CHGNet to generate stable phases with Monte Carlo sampling. Awarded Office of Naval Research grant in 2023 for support.

## TALKS AND POSTERS

---

1. *Capturing Electrochemical Signatures of Real Space Twisted Bilayer Graphene Domains*  
APS Physics, Minneapolis, MN March 2024
2. *Enhanced Electrochemical Activity Volcanoes in Flat-Band Twisted Trilayer Graphene*  
ECS conference, Gothenburg, Sweden Oct 2023
3. *Twisto-electrochemical activity volcanoes in Trilayer Graphene*  
APS Physics, Las Vegas, NV March 2023
4. *Tunable Electrochemistry with Moiré Flat Bands and Topological Defects at Twisted Bilayer Graphene*  
CMU Energy week, Pittsburgh, PA March 2023
5. *Effect of Disorder and Doping on Electronic Structure of  $Li_3V_2O_5$*   
Pittsburgh Quantum Institute Conference, Pittsburgh, PA Sept 2022
6. *Neural Network based Machine Learning Potential for the Lithium Graphite System*  
Gordon Research Seminar and Conference on Batteries, Ventura, CA June 2022
7. *An Accurate Machine Learning Calculator for the Lithium-graphite System*  
CMU MechE symposium, Pittsburgh, PA March 2021
8. *Non-linear Concentration Waves in Current Monitoring Method for Measurement of Electroosmotic Flow*  
APS Fluid Dynamics, Seattle, WA Oct 2019

## INTERNSHIPS

---

1. **Derived pressure oscillation modes of 3D annular-like acoustic cavities using BEM**  
Research scholar, Ohio State University, Columbus, OH May-Jun 2018
2. **Fabricated inkjet printed electromyogram circuit for control of bionic devices**  
Research scholar, Auckland University, New Zealand Nov-Jan 2017-18
3. **Design, fabrication and characterization of liquid cooling vest for summer**  
Summer Undergraduate Research Award, Indian Institute of Technology, Delhi, India May-Jun 2017

## TEACHING

---

1. *Undergraduate Fluid Mechanics*  
Teaching assistant, Pittsburgh, PA Jan-May 2023
2. *Undergraduate Fluid Mechanics*  
Teaching assistant, Pittsburgh, PA Jan-May 2022
3. *Linear Algebra and Differential Equations*  
Teaching assistant, Delhi, India Jan-May 2019
4. *Linear Algebra and Differential Equations*  
Teaching assistant, Delhi, India Aug-Dec 2018

## MENTORING

---

- Supported first year PhD candidate Shravan Godse (CMU) on ONR project for one year Aug-July 2024
- Currently supporting first year PhD candidate Prottay Malakar (Univ. of Michigan) on ONR project Aug 2023

## HONORS AND AWARDS

---

- Travel Grant from American Physical Society GERA Energy workshop March 2024
- Rackham conference travel grant to present research at ECS in Gothenburg, Sweden Aug 2023
- Won best poster award and travel grant from American Physical Society GERA Energy workshop March 2023
- Accepted proposal for Office of Naval Research Award to probe anionic redox in Li-rich cathodes Feb 2023
- Won best poster award at Pittsburgh Quantum Institute conference September 2022
- Won conference travel award from Pittsburgh Quantum Institute May 2022
- Selected to attend Topological Matter School 2021 August 2021
- Won best poster award CMU MechE symposium March 2021
- Ranked in top five students with three semester merit awards in Undergraduate MechE batch August 2019