Mohammad Babar

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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. Efthimios Kaxiras (Havard 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, FEniCS, Quantum Espresso, PyBaMM, GPAW, LAMMPS, Gaussian, Mathematica, Git, Adobe Illustrator
- **Keywords**: Ab Initio · Monte Carlo · Physics-based Simulations · Electronic Structure · Design of Experiments · Density Functional Theory · Machine learning Interatomic Potential · Reaction Kinetics · Batteries · Computational Materials Science · Computational Chemistry · Electrochemistry · Finite Element Analysis

Publications

1. Determining effects of doping lithium nickel oxide with tungsten using Compton scattering (*In Review*)
   V N Kothalawala, ..., **M Babar**, V Viswanathan, H Hafiz, A Bansil
   APL Energy 2 (2) 2024
2. Twisto-electrochemical activity volcanoes in Trilayer Graphene (*In Review*)
   M Babar, Z Zhu, R Kurchin, E Kaxiras, V Viswanathan
   arXiv preprint arXiv:2306.00028 2023
3. 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
4. Effect of disorder and doping on electronic structure and diffusion properties of $Li_3V_2O_5$
   M Babar, H Hafiz, Z Ahmad, B Barbiellini, A Bansil, V Viswanathan
   Journal of Physical Chemistry C, 126, 37, 15549–15557 2022
5. 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
6. 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
7. 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. **Real Space Electrochemical Resolution of Twisted Bilayer Graphene Domains**
   Capturing electrochemical signature of flat bands and resolving domain signals in twisted bilayer graphene by scanning nanopipette over the moiré supercell. Incorporating local density of states in the Gerischer model to obtain steady state voltammograms as a function of twist angle. Solving coupled Poisson and Nernst-Planck equations in FEniCS PDE solver. Manuscript in review.

2. **Magnetic Moment for Fast Redox Analysis in Lithium-rich Transition Metal Cathodes**
   Using total and projected magnetic moments on species over the charge cycles to isolate regions of anionic and cationic redox. Validating and characterizing redox orbitals using Compton scattering spectroscopy through collaborators in Japan. Awarded Office of Naval Research grant in 2023 for support. Expected completion by June 2024.

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 under, Delhi, India — Jan-May 2019
4. *Linear Algebra and Differential Equations*
   Teaching assistant, Delhi, India — Aug-Dec 2018

Mentoring

- Guided first year PhD candidate Shravan Godse (CMU) on ONR project for one year — Aug-July 2024
- Currently advising 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