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: 9.24/10.0 — *Aug 2015 - May 2019*
  Teaching Assistantship: Linear Algebra and Differential equations (2 semesters)

SKILLS SUMMARY

- **Languages**: Python, Julia
- **Tools**: Quantum Espresso, GPAW, LAMMPS, Gaussian 09, FEniCS, MATLAB, SolidWorks, Mathematica, Adobe Illustrator

SELECTED PUBLICATIONS

1. 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

2. 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 — 2023

3. 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

4. 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

5. 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 — 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 revision.

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 May 2024.

HONORS AND AWARDS

- Won best poster award at 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