Mohammad Babar

Website Google Scholar LinkedIn

EDUCATION

University of Michigan

Ann Arbor, MI

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Mobile: +1-412-320-1045

PhD in Mechanical Engineering

Advisor: Dr. Venkatasubramanian Viswanathan

Pittsburgh, PA

Aug 2019 - Dec 2022

Present

Carnegie Mellon University

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

Teaching 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, Gaussian 09, FEniCS, MATLAB, SolidWorks, Mathematica, Adobe Illustrator

SELECTED PUBLICATIONS

ACS Central Science

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.

2023

3. 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

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. Predicting Anionic Redox in Lithium-rich Transition Metal Cathodes

Studying the lithium-rich binary system as cathodes for increasing capacity via anionic (oxygen) redox by substituting 3d transition metals. Validating and characterizing redox orbitals using Compton scattering spectroscopy through collaborators in Japan. Awarded ONR 2023 grant to conduct research for three years.

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

Won best poster award at Pittsburgh Quantum Institute conference

September 2022

Won conference travel award from Pittsburgh Quantum Institute

May 2022

Feb 2023

Selected to attend Topological Matter School 2021

August 2021 March 2021

Won best poster award CMU MechE symposium

August 2019

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

Won Merit Award for three consecutive undergraduate semesters

May 2019