Mohammad Babar

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Education

- **Carnegie Mellon University** — Pittsburgh, PA
  PhD in Mechanical Engineering; GPA: 4.0/4.0 — *Aug 2019 - Present*
  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: Fluid Mechanics, First Year Undergraduate Mathematics (2 semesters)

- **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 $Li_3V_2O_5$
   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 ($Li_2TM_aO_3$-$LiTM_bO_2$) for potential capacity increase through anionic redox by substituting intercalants, transition metals and anions 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

- 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 among 75 students in Undergraduate Mechanical Engineering branch — August 2019
- Won Merit Award for three consecutive undergraduate semesters — May 2019