Zeeshan Ahmad, Ph.D.

Postdoctoral Scholar, Pritzker School of Molecular Engineering, The University of Chicago

Email: azeeshan@uchicago.edu
Web: https://ahzeeshan.github.io Alt: azeeshan@alumni.cmu.edu

Employment

Texas Tech University	Assistant Professor	Aug 2022-
The University of Chicago, Pritzker School of Molecular Engineering	Postdoctoral Scholar Advisor: Dr. Giulia Galli	Sept 2020 - present

Education

Carnegie Mellon University — M.S. & Ph.D. in Mechanical Engineering — 2015-20
Thesis: "Electrolytes for Enabling Rechargeable Lithium Metal Batteries"
Advisor: Dr. Venkat Viswanathan.

Indian Institute of Technology Delhi — B.Tech. in Mechanical Engineering — 2011-15
Thesis: "Droplet formation in a T-junction microfluidic device under electrical actuation"
Advisors: Dr. Amit Gupta & Dr. Supreet S. Bahga. Dept. Rank 1

Research Accomplishments

Ph.D. thesis: *Electrolytes for Enabling Rechargeable Lithium Metal Batteries.*

- Derived generalized design rules for electrode/electrolyte interface stability in solid-state batteries using analytical and computational modeling. Discovered *density-driven* stability regime with soft solid electrolytes
- Performed high-throughput screening of inorganic solids for electrolyte applications based on the developed stability criteria. Employed machine learning to serve as surrogate model for first-principles calculations
- Collaborated with experimentalists to validate the developed theory, confirming the *density-driven* stability mechanism, showing large improvement in Li metal solid-state battery performance at high current densities
- Developed phase-field model for mesoscale simulations of liquid crystalline electrolyte based batteries, connecting device performance to the structure of the electrolyte molecules

Postdoctoral Research: *Theory & Computation for understanding and developing hybrid organic-inorganic semiconductors for energy and computing applications.*

- Quantified electron Rashba spin-orbit coupling effects at the surfaces of lead halide perovskite for solar cell applications, resolving a controversy on the large disparities observed in experiments
- Investigated effects of excess lead iodide precursor on the presence of defects, charge transfer and energy level alignments through first-principles simulations of surfaces and interfaces in perovskite solar cells
- Collaborated with experimentalists within Energy Frontier Research Center to validate the theory and propose new design strategies

Publications

Google Scholar Link: Citations: 618, h-index: 10 (as of Apr 18, 2022)

Peer Reviewed Journal Publications

† denotes equally contributing authors

[J15] **Z. Ahmad**, R. A. Scheidt, M. P. Hautzinger, K. Zhu, M. C. Beard, G. Galli, "Understanding the Effect of Lead Iodide Excess on the Performance of Methylammonium Lead Iodide Perovskite Solar Cells"
ACS Energy Lett., *accepted* arXiv:2201.12473 (2022).

[J14] **Z. Ahmad**, V. Venturi, S. Sripad, V. Viswanathan, "Chemomechanics: friend or foe of the "AND problem" of solid-state batteries?"
Curr. Opin. Solid State Mater. Sci., *accepted*. arXiv:2108.10150 (2022).

[J13] Z. Huang†, S. R. Vardeny†, T. Wang†, **Z. Ahmad†**, A. Chanana, E. Vetter, S. Yang, X. Liu, G. Galli, A. Amassian Z. V. Vardeny, D. Sun, "Observation of Spatially-Resolved Rashba States on the Surface of $CH_3NH_3PbBr_3$ Single Crystals"
Appl. Phys. Rev. 8, 031408 (2021). *Featured Article*

[J12] **Z. Ahmad**, V. Venturi, H. Hafiz, V. Viswanathan, "Interfaces in Solid Electrolyte Interphase: Implications for Lithium-ion Batteries"
J. Phys. Chem. C 125, 11301 (2021).

[J11] A. Mistry $\cdots$ **Z. Ahmad** $\cdots$ V. Viswanathan, "A Minimal Information Set to Enable Verifiable Theoretical Battery Research"
ACS Energy Lett. 6, 3831 (2021). *Battery Modeling Community Article*

[J10] **Z. Ahmad**, Z. Hong, V. Viswanathan, "Design rules for liquid crystalline electrolytes for enabling dendrite-free lithium metal batteries"
Proc. Natl. Acad. Sci. U.S.A. 117, 26672 (2020).

[J9] Z. Hong, **Z. Ahmad**, V. Viswanathan, "Design principles for dendrite suppression with porous polymer/aqueous solution hybrid electrolyte for Zn metal anodes"
ACS Energy Lett. 5, 2466 (2020).

[J8] V. Venturi, H. Parks, **Z. Ahmad**, V. Viswanathan, "Machine learning enabled discovery of application dependent design principles for two-dimensional materials"
Mach. Learn.: Sci. Technol. 1, 035015 (2020).

[J7] C. Fu, V. Venturi, J. Kim, **Z. Ahmad**, A. W. Ells, V. Viswanathan, B. A. Helms, "Universal Chemomechanical Design Rules for Solid-Ion Conductors to Prevent Dendrite Formation in Lithium Metal Batteries"
Nat. Mater. 19, 758 (2020).

[J6] **Z. Ahmad**, T. Xie, C. Maheshwari, J. C. Grossman, V. Viswanathan, "Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Suppression of Dendrite Formation in Lithium Metal Anodes"
ACS Cent. Sci. 4, 996 (2018). *Among 10 Ionizing Papers (August 2018) in Research Interfaces*

[J5] **Z. Ahmad**, V. Viswanathan, "Role of anisotropy in determining stability of electrodeposition at solid-solid interfaces"
Phys. Rev. Materials 1, 055403 (2017).

[J4] **Z. Ahmad**, V. Viswanathan, "Stability of electrodeposition at solid-solid interfaces and implications for metal anodes"
Phys. Rev. Lett. 119, 056401 (2017).

[J3] L. Klosterman, **Z. Ahmad**, V. Viswanathan, C. J. Bettinger, "Synthesis and Measurement of Cohesive Mechanics in Polydopamine Nanomembranes"
Adv. Mater. Interfaces 4, 170041 (2017).

[J2] C. Xu, **Z. Ahmad**, A. Aryanfar, V. Viswanathan, J. R. Greer, "Enhanced strength and temperature dependence of mechanical properties of Li at small length scales and its implications for Li metal anodes"
Proc. Natl. Acad. Sci. U.S.A. 114, 57 (2017).

[J1] **Z. Ahmad**, V. Viswanathan, "Quantification of uncertainty in first-principles predicted mechanical properties of solids: Application to solid ion conductors"
Phys. Rev. B 94, 064105 (2016).

Preprints/Working papers

[PP2] Z. Hong, **Z. Ahmad**, V. Viswanathan, "First principles calculations of surface diffusion barriers on lithium metal: uncertainty qualification and implications for co-electrodeposition", in preparation

[PP1] S. Zhu, Z. Hong, **Z. Ahmad**, V. Viswanathan, "Localized Activity Coefficient-Modulated Recrystallization Phenomenon During Electrodissolution", in preparation

Peer Reviewed Conference Papers

[C2] Y. A. Farrukh, **Z. Ahmad**, I. Khan, R. M. Elavarasan, "A Sequential Supervised Machine Learning Approach for Cyber Attack Detection in a Smart Grid System"
53rd North American Power Symposium, *accepted*. arXiv:2108.00476 (2021).

[C1] **Z. Ahmad**, R. Singh, S. S. Bahga, A. Gupta, "Droplet Formation in a T-Junction Microfluidic Device in the Presence of an Electric Field"
ASME 13th International Conference on Nanochannels, Microchannels and Minichannels (ICNMM) (2015).

Patents

[PT2] V. Viswanathan, **Z. Ahmad**, S. Zhu, "Fast Charging and Discharging Rechargeable Metal Electrode by Isotope Control"
US Patent Application no. 63/054,090 (2020).

[PT1] Y.-M. Chiang, V. Viswanathan, L. Li, V. Pande, D. Krishnamurthy, **Z. Ahmad**, W. H. Woodford, "Lithium metal electrodes and batteries thereof"
US Patent Application no. 15/480,235, granted (2017).

Talks

[T7] (Invited) **Z. Ahmad**, "Solid State Electrolytes for Rechargeable Lithium Metal Batteries"
Battery Modeling Webinar Series (2020).

[T6] **Z. Ahmad**, Z. Hong, V. Viswanathan, "Dendrite Suppression for Metal Anodes Using Liquid Crystalline Electrolytes"
Materials Research Society Fall Meeting (2019).

[T5] **Z. Ahmad**, H. Hafiz, V. Viswanathan, "Design principles for multicomponent solid electrolytes for lithium metal anodes"
American Physical Society March Meeting (2019).

[T4] **Z. Ahmad**, V. Viswanathan, "Solid electrolytes for stable electrodeposition in Li metal anode based batteries"
American Physical Society March Meeting (2018).

[T3] (Invited) **Z. Ahmad**, V. Viswanathan, "Data Science on Inorganic Crystals"
4th Annual Electrochemical Energy Symposium, Carnegie Mellon University (2018).

[T2] **Z Ahmad**, C. Maheshwari, V. Viswanathan, "Machine Learning-Driven Prediction of Electrodeposition Stability of Inorganic Solid Electrolytes with Li-Metal Anode"
Materials Research Society Fall Meeting (2017).

[T1] **Z. Ahmad**, V. Viswanathan, "New Approach of Dendrite Suppression Using Solid Electrolyte to Enable Li Metal Anodes"
Electrochemical Society Fall Meeting (2017).

Poster Presentations

[PS4] **Z. Ahmad**, V. Viswanathan, "Development of solid ion conductors for stable electrodeposition at electrolyte-Li metal anode interfaces"
Batteries Gordon Research Conference (2018).

[PS3] **Z. Ahmad**, V. Viswanathan, "Solid-Solid Interfaces for Suppression of Dendrites in Metal Anode Based Batteries"
Materials Research Society Fall Meeting (2017).

[PS2] **Z. Ahmad**, V. Viswanathan, "Data-driven Computational Screening of Stable Solid Ion Conductors for Li Anode-based Batteries"
Science 2017 Conference, University of Pittsburgh (2017). **Best Poster Award**

[PS1] **Z. Ahmad**, V. Viswanathan, "Tin as Anode Material for Lithium-ion batteries"
1st Annual Electrochemical Energy Symposium, Carnegie Mellon University (2015). **Best Poster Award**

Awards and Fellowships

American Physical Society Energy Research Workshop Travel Award, 2019.

Bushnell Fellowship in Engineering, Carnegie Mellon University, for doctoral research in nanotechnology, 2018.

Phillips and Huang Family Fellowship in Energy, Carnegie Mellon University, 2016.

Institute Silver Medal at IIT Delhi, for graduating at the top of the department batch, 2015.

Nayyar Perwez Shahabuddin Medal at IIT Delhi, awarded for research record and potential, 2015.

Institute Semester Merit Prize (six times) at IIT Delhi, 2012-2015.

IIT Delhi Alumni Association Scholarship for excellent academic record, 2013 & 2014.

Jagdishwar & Maya Jaluria Scholarship at IIT Delhi, 2013 & 2014.

S.C. Mehrotra's Award at IIT Delhi, 2013.

Kishore Vaigyanik Protsahan Yojana (KVPY) Fellowship by Govt. of India, 2011.

Teaching Experience

Teaching Assistant	Fluid Mechanics (undergraduate), Carnegie Mellon University	Spring 2018 & 2019

Training, Mentoring & Advising Experience

Mohd Babar, Ph.D. student, CMU		2021-
Shang Zhu, Ph.D. student, CMU		2019-
Victor Venturi, Ph.D. student, CMU		2017-2020
Chinmay Maheshwari, undergrad intern, CMU	Post-grad: Ph.D. student, UC Berkeley	2017
Ashwini Gupta, undergrad intern, CMU	Post-grad: Ph.D. student, Johns Hopkins	2016

Academic Service

- Reviewer
  - Journals: Physical Review Letters, Journal of the American Chemical Society, Physical Review X, Physical Review B, Physical Review Materials, Journal of Physics: Condensed Matter, Journal of Applied Physics, Computational Materials Science, Machine Learning: Science and Technology, Scientific Data
  - Conferences: NeurIPS (Machine Learning & the Physical Sciences Workshop, 2019 & 2020)

  - Poster Judge for Pittsburgh Quantum Institute

- University
  - Graduate Student Representative, Carnegie Mellon Graduate Student Assembly (2018 - 2019).
  - Member, Campus Affairs Committee (2018 - 2019). Working group focused on mental health, workplace bullying & graduate student housing
  - Logistics Secretary, Mechanical Engineering Society, Indian Institute of Technology Delhi (2013-14).

Additional Training

Quantum Matters in Materials Science Workshop, National Insitute of Standards and Technology (virtual), 2020

Artificial Intelligence for Materials Science Workshop, National Insitute of Standards and Technology, 2019

International Summer School on Computational Quantum Materials, University of Sherbrooke, 2018

SUNCAT Summer Institute: Fundamentals and Applications of Heterogeneous Catalysis, Stanford University, 2017

Selected Media Coverage

- Phys.org: The surprising strength of liquid crystals, Nov 3, 2020 (`https://phys.org/news/2020-11-strength-liquid-crystals.html`).
- CleanTechnica: The Key To Better Batteries Is Soft Solid Electrolytes, Say Researchers, July 22, 2020 (`https://cleantechnica.com/2020/07/22/the-key-to-better-batteries-is-soft-solid-electrolytes-say-researchers`)
- HPC Wire: CMU Scientists Use XSEDE-Allocated Resources to Simulate Improved Battery Components, July 11, 2019 (`https://www.hpcwire.com/off-the-wire/cmu-scientists-use-xsede-allocated-resources-to-simulate-improved-battery-components/`).
- Techxplore: Machine learning to develop safer batteries, Dec 18, 2018 (`https://techxplore.com/news/2018-12-machine-safer-batteries.html`).
- Techxplore: Building better batteries, Dec 20, 2016 (`https://techxplore.com/news/2016-12-batteries.html`).