

Zeeshan Ahmad, Ph.D.

Assistant Professor, Mechanical Engineering, Texas Tech University

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Employment

Assistant Professor	Mechanical Engineering, Texas Tech University	09/2022-present
Postdoctoral Scholar	Pritzker School of Molecular Engineering, University of Chicago	09/2020-08/2022
	Advisor: Dr. Giulia Galli	

Education

Carnegie Mellon University	M.S. & Ph.D. in Mechanical Engineering	2020
	Thesis: “Electrolytes for Enabling Rechargeable Lithium Metal Batteries”	
	Advisor: Dr. Venkat Viswanathan.	
Indian Institute of Technology Delhi	B.Tech. in Mechanical Engineering	2015
	Thesis: “Droplet formation in a T-junction microfluidic device under electrical actuation”	
	Advisors: Dr. Amit Gupta & Dr. Supreet S. Bahga. Dept. Rank 1	

Research Expertise

Materials Theory (Quantum Mechanical, Continuum Scale Modeling) & Electrochemical Characterization for Next-generation Batteries, Photovoltaic, & Optoelectronic Applications
Machine Learning for Materials Science

Publications

Google Scholar Link: Citations: 1598, h-index: 17 (as of June 2025)

† denotes equally contributing authors

Preprints

- [PP1] **Z. Ahmad**, “Equivariant Machine Learning Interatomic Potentials with Global Charge Redistribution”
arXiv preprint arXiv:2503.17949 (2025)

Peer Reviewed Journal Publications

- [J24] **Z. Ahmad**, “A Unified and Consistent Electrical Double Layer Model for Treatment of Core and Space Charge Layer in Solid Electrolytes”
J. Mater. Chem. A, *accepted* (2025).
- [J23] S. R. Mohanty, M. U. Maruf, V. Singh, **Z. Ahmad**, “Machine learning approaches for automatic defect detection in photovoltaic systems”
Solar Energy 298, 113672 (2025).
- [J22] M. S. R. Limon, C. W. Duffee, **Z. Ahmad**, “Constriction and Contact Impedance of Ceramic Solid Electrolytes”
ACS Energy Letters 10, 1999 (2025).
- [J21] B. Wang, M. S. R. Limon, Y. Zhou, K. Cho, **Z. Ahmad**, L. Su, “ $1 + 1 > 2$ Effect Induced by Space Charge in Solid Electrolytes”
ACS Energy Letters 10, 1255 (2025). *Selected for cover art*

- [J20] B. Ahmad, M. S. R. Limon, **Z. Ahmad**, “Modulation of Point Defect Properties Near Surfaces in Metal Halide Perovskites”,
Phys. Rev. Materials 8, 125402 (2024).
- [J19] M. S. R. Limon, **Z. Ahmad**, “Heterogeneity in Point Defect Distribution and Mobility in Solid Ion Conductors”,
ACS Applied Mater. Interfaces 16, 50948 (2024).
- [J18] F. Lv, Z. Hong, **Z. Ahmad**, H. Li, Y. Wu, Y. Huang, “Design of Flexible Piezoelectric Nanocomposite for Energy Harvesters: A Review”
Energy Mater. Adv. 4, 0043 (2023).
- [J17] S. Zhu, Z. Hong, **Z. Ahmad**, V. Viswanathan, “Localized Recrystallization of a Lithium-Metal Anode during Fast Stripping in High-Activity Liquid Electrolytes”
ACS Appl. Mater. Interfaces 15, 6639 (2023).
- [J16] M. Babar, H. Hafiz, **Z. Ahmad**, B. Barbiellini, A. Bansil, V. Viswanathan, “Effect of disorder and doping on electronic structure and diffusion properties of $\text{Li}_3\text{V}_2\text{O}_5$ ”
J. Phys. Chem. C, 126, 15549 (2022).
- [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. 7, 1912 (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. 26, 101002 (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 $\text{CH}_3\text{NH}_3\text{PbBr}_3$ 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 ... **Z. Ahmad** ... 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).

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. 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. 17/927,455 (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

- [T11] (Invited) **Z. Ahmad**, “AI for materials discovery”
Zu-Grama DeepTech/AI week (2025).
- [T10] (Invited) **Z. Ahmad**, “The electrical double layer in solid-state batteries”
Department of Chemistry and Biochemistry, Texas Tech University (2025).
- [T9] **Z. Ahmad**, Y. Shin, G. Galli, “Modulating defects in metal halide perovskites using lattice strain”
American Physical Society March Meeting (2023).
- [T8] **Z. Ahmad**, G. Galli, “Surface and interfacial heterogeneities in hybrid perovskite solar cells,”
American Physical Society March Meeting (2022).
- [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).

Awards and Fellowships

WelchX Collaboration Retreat Invitee for theme: Chemical Research for Grand Challenges, 2025

Class of Influential Researchers by American Chemical Society Industrial & Engineering Chemistry Research, 2025

Emerging Investigators in Electrochemical Energy Conversion and Storage for ASME Journal of Electrochemical Energy Conversion and Storage, 2025

Samsung Global Research Outreach Award, 2023

American Physical Society Energy Research Workshop Travel Award, 2023 & 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

Course Instructor	Engineering Thermodynamics I (undergraduate), Texas Tech University	6 semesters
Teaching Assistant	Fluid Mechanics (undergraduate), Carnegie Mellon University	2 semesters

Training, Mentoring & Advising Experience

PhD students

Md Salman Rabbi Limon	9/22 -
Moin Uddin Maruf	1/24 -
Abrar Fahim Navid	6/24 -

Master's students

Bilal Ahmad	graduated	9/23 - 12/24
Muhammad Zain Sarwar		1/25 -
Anibesh Dhamala		9/22-12/24

Undergraduate students

Curtis Duffee	9/23 -
Muhammad Abid Inam	1/25 -
Worth Lacy	9/24 -
Thong Duong	9/24 -
Philip Onischuk	9/23 - 6/24

Academic Service

- Session Chair
 - American Physical Society March Meeting (2023)
- Reviewer
 - Grant reviewer, NASA
 - Journals: Physical Review Letters, ACS Energy Letters, Journal of the American Chemical Society, Physical Review X, PRX Energy, 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, Energy Material Advances, Journal of Electrochemical Energy Conversion and Storage
 - Conferences: NeurIPS (Machine Learning & the Physical Sciences Workshop, 2019 & 2020)
 - Poster Judge for Pittsburgh Quantum Institute
- University
 - Graduate Education Committee, TTU Mechanical Engineering (2024-)
 - Undergraduate curriculum committee, TTU Mechanical Engineering (2023-2024)
 - Qualifying Exam Committee (Solid mechanics), TTU Mechanical Engineering (2022)
 - Graduate Student Representative, CMU Graduate Student Assembly (2018 - 2019).
 - Member, CMU Campus Affairs Committee (2018 - 2019).
 - Logistics Secretary, Mechanical Engineering Society, Indian Institute of Technology Delhi (2013-14).

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-xse-de-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>).