



TEXAS TECH UNIVERSITY

Edward E. Whitacre Jr.  
College of Engineering

Department of Mechanical Engineering

## Design of Functional Materials and Interfaces for Energy Storage and Conversion

Dr. Zeeshan Ahmad

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

A drastic switch to renewable energy conversion and storage technologies is required to meet the decarbonization goals of the Paris agreement. There remain challenges related to the energy density, conversion efficiency, cost, integration, and scaleup of emerging renewable technologies. Materials are at the forefront of these challenges and provide a promising route to enable these technologies allowing beyond incremental progress on relevant metrics. This talk will discuss how a combination of theory, computation, and data-driven methods can accelerate the design of functional materials and interfaces for solid-state lithium metal batteries. I will describe the manipulation of the coupling between mechanics and electrochemistry to mitigate the challenges associated with high energy density solid-state batteries. By incorporating the modification of the electrochemical kinetics due to mechanical stresses developed in the solid electrolyte, we identify a new paradigm of stability based on soft solid electrolytes that can lead to uniform electrodeposition. This regime is experimentally confirmed using a composite solid electrolyte designed such that its mechanical properties lie in the stability region. We further couple our design criteria with a machine learning framework for inorganic crystals to screen tens of thousands of candidates, resulting in the discovery of new solid electrolytes in a fraction of the time required by density functional theory calculations.

### Bio Sketch

Dr. Zeeshan Ahmad is a postdoctoral scholar at the Pritzker School of Molecular Engineering, University of Chicago. His research aims to advance renewable energy and electrify transportation through fundamental understanding and design of materials for batteries and solar photovoltaics. He received his B. Tech. in Mechanical Engineering from the Indian Institute of Technology (IIT) Delhi in 2015 and his M.S. and Ph.D. in Mechanical Engineering from Carnegie Mellon University in 2020. He has been the recipient of numerous awards such as the Institute Silver Medal at IIT Delhi, the Bushnell Fellowship in Engineering and the Phillips and Huang Family Fellowship in Energy at Carnegie Mellon University.

Department of Mechanical Engineering, Edward E. Whitacre Jr. College of Engineering

Monday, Feb 28, 2022

2:00 – 3:00 PM

In person: ME South 205

Online:

<https://texastech.zoom.us/j/94591486607?pwd=MHhsSnJyM2RJQjl1ZmduWkZuVExrQT09>

Meeting ID: 945 9148 6607 Passcode: 844848