SCHOOL OF MECHANICAL & MATERIALS ENGINEERING

GRADUATE SEMINAR SERIES

Atomistic Modelling of Solid-State Electrolytes for Sodium-Ion Batteries

Presented by

Aniruddha Dive, Ph.D. candidate in Mechanical Engineering

Abstract

Limited lithium reserves and ever-increasing energy demands have intensified the need for economical alternatives. The natural abundance of sodium makes sodium-ion batteries a promising alternative, especially for grid energy storage. Conventional liquid electrolytes pose safety concerns due to poor stability, which has led to an extensive research to explore solid-state electrolytes. Developing novel solid electrolytes with ionic conductivity comparable to that of liquid electrolytes has been a major challenge over the past decade. Sulfide glasses have been reported to possess excellent ionic conductivity making them potential electrolytes for high performance sodium-ion batteries. Optimizing electrolyte compositions through series of fabrication and experimental characterization cycles is not an economical approach. Atomistic simulations provide an economical route to analyze wide range of compositions and get crucial insights into ion transport within these glasses. With this motivation, the seminar will provide an overview of atomistic modelling efforts to investigate the local structure of the glasses and correlate it to the ion transport within these glasses.

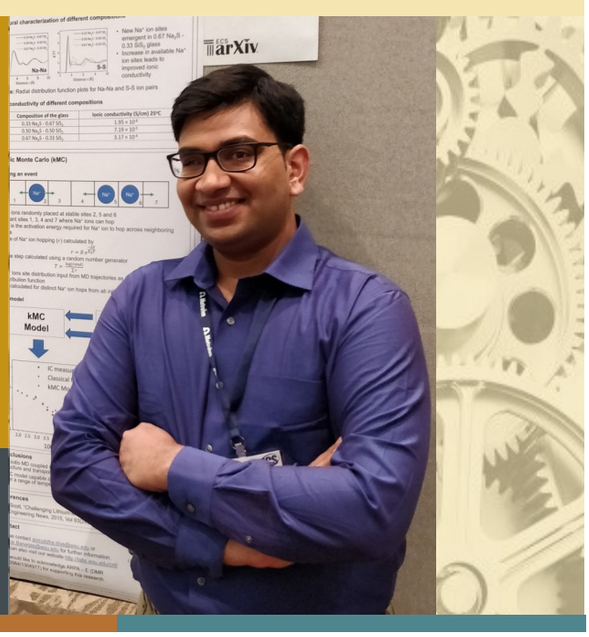
The seminar focusses on the modeling of sodium thiosilicate [x Na_2S – (1-x) SiS_2] glasses employing both *ab initio* as well as classical molecular dynamics (MD) simulation techniques. We validated our MD simulations by calculating the overall static structure factors S(Q) from *ab initio* MD and compared it to those obtained through X-ray scattering experiments. Our calculations provide critical insights into ion transport through these glasses, reporting an optimal room temperature ionic conductivity of ~ 10^{-4} S/cm for 67 Na_2S – 33 SiS_2 composition. We have also modeled sodium thiophosphate glasses [x Na_2S – (1-x) P_2S_5] reporting an optimal ionic conductivity of ~ 10^{-5} S/cm for 75 Na_2S – 25 P_2S_5 glass. These novel atomistic modeling techniques provide an economical route for understanding the ion transport in complex glasses and thereby assist in designing novel electrolytes for sodium-ion batteries.

Biography

Aniruddha Dive is a Ph. D. candidate in Mechanical Engineering at Washington State University. His current research involves investigating ion transport in electrolytes and across electrolyte-electrode interfaces for energy storage devices using atomistic modeling techniques. He received his B. Tech. in Metallurgy and Materials Engineering from Visvesvaraya National Institute of Technology (VNIT), India in 2010. He received his M. Tech. in Materials Science from Indian Institute of Technology (IIT), Kharagpur, India in 2012. After his graduation he has worked in electric vehicles industry from 2012-2014. He started working in Computational Nanomaterials Lab at WSU from Spring 2015.

Thursday, January 24, 2019
11:00am to Noon
ETRL room 101

Meet the speakers before the seminar in ETRL room 119, 10:30am to 10:50am. Light refreshments will be served.



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