

**MATERIALS ENGINEERING
SEMINAR**

“A Quest for Better Battery Materials: Accelerating Discovery Through Efficient Exploration and Rational Design”

**By
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Purdue MSE Ph.D. Final Exam

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ABSTRACT

The Materials Genome Initiative (MGI) has established guidelines to accelerate the discovery, development, and implementation of advanced materials in order to address current and future challenges. A key area of interest is the pressing need for more efficient energy storage systems to support technologies such as electric vehicles and renewable energies. In this work, we present an Integrated Computational Materials Engineering approach for the development of novel solid-state electrolyte materials. In particular, we embark on a quest to unravel the potential of ceramic garnet lithium lanthanum zirconium oxide (LLZO) for next-generation battery technologies.

Our exploration begins with an overview of the current state of the Materials Innovation Infrastructure and our rationale behind choosing LLZO. Through the use of machine learning techniques and molecular dynamics simulations, we aim for efficient material optimization. Our findings are reinforced through experiments by using these materials as inorganic fillers in composite polymer electrolytes. Our findings demonstrate that the combined use of these complementary techniques facilitates the discovery of potential alternative solid-state electrolytes. Finally, we propose future research directions in materials science for the design of advanced materials using these integrated approaches.

Date: Friday, July 14th, 2023

Time: 12:30 P.M.

Place: DLRC 131 or <https://purdue.webex.com/join/strachan>



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