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Collaborative Data Refinement for Enhanced Ionic Conductivity Prediction in Garnet-Type Materials

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Abstract : Solid-state lithium-ion batteries have garnered increasing interest in modern energy research due to their potential for safer, more efficient, and sustainable energy storage systems. Among the critical components of these batteries, the electrolyte plays a pivotal role, with LLZO garnet-based electrolytes showing significant promise. Garnet materials offer intrinsic advantages such as high Li-ion conductivity, wide electrochemical stability, and excellent compatibility with lithium metal anodes. However, optimizing ionic conductivity in garnet structures poses a complex challenge, primarily due to the multitude of potential dopants that can be incorporated into the LLZO crystal lattice. The complexity of material design, influenced by numerous dopant options, requires a systematic method to find the most effective combinations. This study highlights the utility of machine learning (ML) techniques in the materials discovery process to navigate the complex range of factors in garnet-based electrolytes. Collaborators from the materials science and ML fields worked with a comprehensive dataset previously employed in a similar study and collected from various literature sources. This dataset served as the foundation for an extensive data refinement phase, where meticulous error identification, correction, outlier removal, and garnet-specific feature engineering were conducted. This rigorous process substantially improved the dataset's quality, ensuring it accurately captured the underlying physical and chemical principles governing garnet ionic conductivity. The data refinement effort resulted in a significant improvement in the predictive performance of the machine learning model. Originally starting at an accuracy of 0.32, the model underwent substantial refinement, ultimately achieving an accuracy of 0.88. This enhancement highlights the effectiveness of the interdisciplinary approach and underscores the substantial potential of machine learning techniques in materials science research.

Keywords : lithium batteries, all-solid-state batteries, machine learning, solid state electrolytes
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