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Unveiling Key Factors and Design Implications for Enhancing Li Diffusion in Garnet Ionic Conductors

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This study presents data-driven insights into the key factors influencing Li diffusion in garnet ionic conductors and their implications for design and optimization. Understanding and enhancing Li diffusion in these materials is crucial for advancing energy storage technologies. Descriptors related to structure, composition, atomic environment, conduction pathway, and substitution are employed to analyze Li diffusion in garnet structures. Through extensive correlation analysis, we establish a clear relationship between Li ionic conduction and important factors, including Li concentration, Li occupancy (96h), and substitution at A (24d) and D (16a) sites. Additionally, we observe that heterovalent disorder resulting from A site substitution affects the atomic environment of Li ions, while sublattice disorder through D site substitution influences the Li-Li distance. These data-driven findings offer valuable insights for optimizing the design and synthesis of garnet ionic conductors with enhanced conductivity. Future investigations may focus on further experimental validation and the development of strategies to improve Li diffusion and conductivity, thereby paving the path for progress in the field of ionic conductors and their application in energy storage systems.