$Li_3OCl|Li$ Interfaces for Solid-State Batteries: A Defect-Engineering Study

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The performance of solid-state lithium-metal batteries is critically influenced by the interface between the solid electrolyte and lithium metal. Li_3OCl antiperovskite electrolytes offer attractive ionic transport properties, yet their application is limited by interfacial instability and suboptimal lithium transport. In this study, we investigate the $Li_3OCl|Li$ interface using first-principles calculations, with a focus on defect engineering in the Li_3OCl solid electrolyte. Explicit atomistic interface models are constructed to examine interfacial structure, energetics, and charge redistribution. Intrinsic lithium defects are introduced to assess their impact on bulk and interfacial behavior. The results show that defect engineering can significantly improve lithium affinity and reduce interfacial energy while enhancing ion transport pathways and maintaining electronic insulation. These findings provide practical atomic-scale insights into stabilizing $Li_3OCl|Li$ interfaces and highlight defect engineering as an effective strategy for advancing solid-state lithium-metal battery technologies.