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First Principles Studies for Lithium Intercalation and Diffusion Behaviors in MoS2 treated with the Compressive Sensing Cluster Expansion CHI-PING LIU, FEI ZHOU, VIDVUDS OZOLINS, University of California, Los Angeles, California — Molybdenum disulfide (MoS2) is a good candidate electrode material for high capacity energy storage applications, such as lithium ion batteries and supercapacitors. In this work, we investigate lithium intercalation and diffusion kinetics in MoS2 by using first-principles density-functional theory (DFT) calculations. Two different lithium intercalation sites (1-H and 2-T) in MoS2 are found to be stable for lithium intercalation at different van der Waals' (vdW) gap distances. It is found that both thermodynamic and kinetic properties are highly related to the interlayer vdW gap distance, and that the optimal gap distance leads to effective solid-state diffusion in MoS2. Additionally, through the use of compressive sensing, we build accurate cluster expansion models to study the thermodynamic properties of MoS2 at high lithium content by truncating the higher order effective clusters with significant contributions. The results show that compressive sensing cluster expansion is a rigorous and powerful tool for model construction for advanced electrochemical applications in the future.

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