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Compressive Sensing Cluster Expansion Studies of Lithium Intercalation and Phase Transformation in MoS2 for Energy Storage CHI-PING LIU, University of California, Los Angeles, FEI ZHOU, Lawrence livermore national laboratory, VIDVUDS OZOLINS, University of California, Los Angeles, UNIVERSITY OF CALIFORNIA, LOS ANGELES COLLABORATION, LAWRENCE LIVERMORE NATIONAL LABORATORY COLLABORATION — Bulk molybdenum disulfide (MoS2) is a good electrode material candidate for energy storage applications, such as lithium ion batteries and supercapacitors due to its high theoretical energy and power density. First-principles density-functional theory (DFT) calculations combined with cluster expansion are an effective method to study thermodynamic and kinetic properties of electrode materials. In order to construct accurate models for cluster expansion, it is important to effectively choose clusters with significant contributions. In this work, we employ a compressive sensing based technique to select relevant clusters in order to build an accurate Hamiltonian for cluster expansion, enabling the study of Li intercalation in MoS2. We find that the 2H MoS2 structure is only stable at low Li content while 1T MoS2 is the preferred phase at high Li content. The results show that the 2H MoS2 phase transforms into the disordered 1T phase and the disordered 1T structure remains after the first Li insertion/deinsertion cycle suggesting that disordered 1T MoS2 is stable even at dilute Li content. This work also highlights that cluster expansion treated with compressive sensing is an effective and powerful tool for model construction and can be applied to advanced battery and supercapacitor electrode materials.

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