**Electrochemical Performance of Layered-Expanded Metal Dichalcogenides Cathodes for Mg-ion Batteries**

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**Abstract**

Rechargeable Mg-ion batteries (MIBs) have become a plausible alternative to Li-ion batteries (LIBs) in terms of energy density, scalability and operation safety.1-3 This stems from the fact that Mg metal behaves as a promising anode with high abundance in earth crust, high volumetric capacity, low redox potential (-2.37 V vs SHE), and highly reversible dendrite-free deposition. To fulfill the practical application of Mg metal anode in MIBs, great efforts have been devoted in the search of high performance cathode candidates. Recently, layered metal chalcogenides (i.e. MoS2 and TiS2) have been experimentally explored as high energy-density cathode materials for MIBs.4-6 However, the underlying mechanisms of Mg intercalation into these layered cathodes are still well understood. In this work, we carry out first-principles calculations to investigate electrochemical performance of layered MoS2 and TiS2 cathodes, as well as corresponding phase transition (such as hexagonal to tetragonal) during Mg intercalation. We also study the effect of interlayer spacing on battery performance (i.e. voltage performance and specific capacity) of layered MoS2 and TiS2 cathodes. Our theoretical predictions and understanding of electrochemical performance of layered metal dichalcogenides cathodes can inspire optimal designs of promising layered cathodes for Mg-ion batteries.

**References**

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