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Possible Mg intercalation mechanism at the Mo6S8 cathode surface proposed by first-principles methods[1] LIWEN WAN, DAVID PRENDERGAST, Joint Center for Energy Storage Research, The Molecular Foundry, Lawrence Berkeley National Laboratory — In recent years, great attention has been paid to the development of divalent Mg-ion batteries, which can potentially double the energy density and volumetric capacity compared to monovalent Li-ion batteries. The prototype Mg-ion battery, comprising Mg(anode)/$Mg(AlCl_2BuEt)_2$·THF(electrolyte)/Mo_6S_8(cathode), was established in 2000 by Aurbach et al. Despite the remarkable success of this prototype system, we still lack a clear understanding of the fundamental Mg intercalation/deposition mechanism at the electrolyte/electrode interfaces that perhaps results in the observed sluggish Mg transport process. Our previous work has shown that Mg-ions are strongly coordinated in the bulk electrolyte by a combination of counterion, Cl^-, and organic aprotic solvent, THF. In this work, we use first-principles methods to study Mg intercalation behavior at the Mo_6S_8 cathode surface with the presence of solvent molecules. It is found that the image charge, formed on this metallic cathode surface, can effectively weaken the solvent-surface interactions and facilitate Mg intercalation. A detailed Mg intercalation mechanism is proposed and the unique role of Mo_6S_8 as the cathode material is emphasized.

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