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Understanding the good kinetics of Mo_6S_8 as cathode in Mg ion batteries by key electronic states. PENGFEI YU, Lawrence Berkeley Laboratory, FUDONG HAN, University of Maryland, NIAN ZHANG, XINGHUI LONG, XUEFEI FENG, Chinese Academy of Sciences, CHUNSHENG WANG, University of Maryland, XIAOSONG LIU, ZHI LIU, Chinese Academy of Sciences, CHENG WANG, Lawrence Berkeley Laboratory, CHENG WANG COLLABORATION, CHUNSHENG WANG TEAM — Up to now, Chevrel phase ($Mo_6X_nX'_{8-n}$, X=S, X'=Se) is still the unique cathode material in Mg ion batteries that has acceptable kinetic performance. However, the origin of good kinetics still needs to be clarified for further, which is critical to the rational explore of the cathode material for the battery with both good cycling performance and specific energy, though some studies have been investigated from the point view of electrochemistry and crystal structure. The study on electronic structure is eager to get a deep insight of the intrinsic property due to the $2e^-$ charge transfer in Chevrel phase and the inspiration from the success studies of the key electronic states in lithium ion batteries. In this report, the unoccupied states of a typical Chevrel phase Mo_6S_8 including Mo L-edge and S K-edge were studied with various amount of Mg^{2+} inserted by tender X-ray absorption spectroscopy. A key electronic state at the pre-edge of S spectra were found to be evolved regularly with Mg^{2+} inserted and extracted. It is assigned to be hybridization between Mo 4d states and S 3p states. The evolution of this state opens a gate to reveal the nature of good kinetics in Chevrel phase.

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