An integrated investigation of the Rate-Liming Step in $Li_4Ti_5O_{12}$ defect spinel anode materials for Lithium-Ion Batteries

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The $Li_4Ti_5O_{12}$ (LTO) defect spinel is a promising anode material for lithium-ion batteries (LIBs) because of its negligible volume change and stable operating voltage during charge and discharge. However, LTO's intrinsic insulating character and moderate ionic transport result in low-rate capability and hinders its high-power applications. Considerable approaches to enhance the rate capabilities of LTO have been carried out, such as compositing by incorporation of conductive agents, doping of metals ions, and surface modification. Applying combinations of the above approaches without a definitive understanding of the individual contributions does not answer the central question for LTO: the rate-limiting step. Here, we investigated the effects of metal doping and carbon coating on LTO to reveal their contributions to the rate enhancements and the rate-limiting step in LTO by integrating *ab initio* calculations and experimental validation. The phase stability, electronic conductivity and Li ion diffusivity of the simple metal-doped LTO (M = Na, K, Mg, Ca, Sr, Al, and Ga) and transition metal-doped LTO (M=Zr, Nb, Ta, Cr, Mo, W, Mn, Fe, Co, Ni, and Cu) as well as the interfacial kinetics of m-RAPET [1] LTO are investigated. The integrated investigations provide insights into the electrochemical kinetical of LTO and the understanding of the ion doping and carbon coating suggests the desired approaches for LTO.

References:

[1] R.N Nasara, P-C. Tsai, S-K Lin, Adv. Mater. Interfaces 2017, 1700329