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Discharge reaction mechanism in SnS anode for Na-ion batteries: First-principles calculations HIROKI KOTAKA, ESICB, Kyoto University, HIROYOSHI MOMIDA, TAMIO OGUCHI, ISIR, Osaka University — Li-ion batteries have been widely used as power sources in modern electronics devices because of its high energy densities and high voltages. However typical Li-ion batteries are relatively expensive, because electrode materials contain high-cost rare-metals such as Li and Co. To solve the cost problem, Na-ion batteries have been recently expected as a next-generation rechargeable battery in which high-cost Li is replaced with low-cost Na. As an anode material suitable for Na-ion batteries, beta-Sn is known to show a high energy density, but one problem of Sn anode is very large volume changes during charge and discharge processes. In this study, we focus attention on tin sulfide (SnS) as a candidate anode material for Na-ion batteries. We perform structural searches of possible reaction products during discharge reaction processes, and theoretically find the discharge reaction formulae for the Na-SnS half-cell by using the first-principles calculations. We show the electrochemical properties such as voltage-capacity curves, and compare our calculated results with the experiments. We also show calculation results of x-ray absorption spectra, and discuss the experimentally reported spectral changes during discharging.

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