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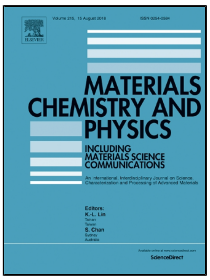

Surface Magnesiation of Tin and Bismuth as Anode Materials of for Magnesium Ion Batteries

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ABSTRACT: Electrochemical behaviour can be improved by decreasing the size of anode materials. In this work, the surface stability, surface adsorption and surface intercalation of nanoscale β-tin (β-Sn) and bismuth (Bi) as anode materials for magnesium (Mg) ion batteries (MIBs) were studied using first-principle calculations. The results show that the (100) and (111) surfaces are energetically stable for β-Sn and Bi, respectively. The diffusion of Mg from the surface to the inside through the Sn (100) surface was not affected by the appearance of the surface, whereas a rate-liming step appears for the Mg diffusion from the surface to the subsurface in Bi. Surface modification is necessary to improve the electrochemical behaviour of Bi as an anode for MIBs.

KEYWORDS: Surface magnesiation; Magnesium ion batteries; Sn and Bi; Anode materials; First-principle calculations