Tin Monoxide Monolayer as Promising Anode Materials for Recharge Ion Batteries

Aijian Huang, Xiaoli Sun^{*}, Sha Dong

School of Physical Electronics, University of Electronic Science and Technology of China, Chengdu, 610054, P.R. China

^{*}E-mail: 201511040202@std.uestc.edu.cn

doi: 10.20964/2017.11.08

Received: 22 July 2017 / Accepted: 28 August 2017 / Published: 12 October 2017

Using density functional theory, Li, Na and Mg adsorption and diffusion on a SnO monolayer were investigated. The energetically favored adsorption sites and diffusion paths for Li, Na and Mg were determined. The adsorption energies were in the range of -1.25 ~ -0.94 eV, -0.99 ~ -0.78 eV, and -1.11 ~ -0.66 eV for Li, Na and Mg adsorption with concentrations between $x=0.03125$ -1.0 in $M_x\text{SnO}$ ($M=\text{Li, Na, or Mg}$). The volume evolutions were within -4% ~ 8% after Li, Na and Mg adsorption. The smallest energy barriers were 0.31, 0.24 and 0.21 eV for Li, Na and Mg, respectively, diffusing on the SnO monolayer. The SnO monolayer showed strong adsorption stability and low Li, Na and Mg diffusion energy barriers with small volume deformations. Therefore, the SnO monolayer is a promising anode material for rechargeable ion batteries.

Keywords: Monolayer SnO, LIBs, NIBs, MIBs, adsorption energy, diffusion energy

[FULL TEXT](#)

© 2017 The Authors. Published by ESG (www.electrochemsci.org). This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).