

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

High ionic conductivity NASICON based materials for Na-ion batteries: a density functional approach K. M. BUI, NIMS, V. A. DINH, Osaka Univ., S. OKADA, Tsukuba Univ., T. OHNO, NIMS — Sodium ion batteries are now believed to be the best candidate for large-scale applications. Simultaneously, it is required to develop solid-state batteries using solid electrolytes for advancing the safety and reliability of batteries. The most promising solid-state battery is composed of the 3-D NASICON electrode $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ (NVP) and electrolyte $\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$ (NZSP). In this work, we aim to theoretically investigate the structures and the diffusion pathway of Na in these materials. Using density functional theory (DFT) method, we investigated the structures and diffusion mechanism of Na ions in the materials. They are insulators with large band. The polaron formation is found to occur only in NVP. Na ions can diffuse along three preferable diffusion pathways; those are, two intra-layer and one inter-layer pathway that takes place between Na layers via the empty Na site. In accordance with experiments reported before, the materials have high ionic conductivity with the activation barrier of about 760meV and 370meV for NVP and NZSP, respectively.

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Date submitted: 14 Nov 2014

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