

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Electronic structures of superionic conductor Li_3N MASARU AOKI, Shizuoka Sangyo University, YOSHIYUKI ODE, KAZUO TSUMURAYA, Meiji University — Lithium nitride is a superionic conductor with high Li conductivity. The compound has been studied extensively because of its potential utility as electrolyte in solid-state batteries. Though the mobility of the cations within the crystalline solid is high comparable to that of molten salts, the mechanism of the high mobility of the cations remains unsolved. To clarify the origin of the mobility we investigate the electronic states of the Li cations in the Li_3N crystal with the first principles electronic structure analysis, focusing a correlation between the cations and the ionicities of the constituent atoms. We have found the existence of the covalent bonding between the Li atoms in the Li_3N crystal in spite of the ionized states of the constituent atoms.

Masaru Aoki
Shizuoka Sangyo University

Date submitted: 19 Nov 2010

Electronic form version 1.4