

Abstract Submitted
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**Indirect correlation between superionic sodiums in β -alumina -
First principles molecular dynamic study-** KAZUO TSUMURAYA, SHOICHI
YASUDA, Meiji University, Kanagawa Japan — The atoms are ionized in the ion
conductors like the atoms in the ionic crystals, yet either cations or anions are mobile
under the electric field unlike the ions in the ionic crystals. The elucidation of the
conduction mechanism is essential for the development of the secondary batteries
which operate at low temperature. Since the Na-Na correlation peak in superionic
 β -alumina has been located at a well separated from the peak position arising from
the commensurate sites, the analyses of the origin of the correlation peak allows us
to give the nature of the conduction mechanism in conductors. The first principles
molecular dynamic study shows that split-interstitial sodiums on mid-oxygen pro-
duce the correlation. This is an indirect correlation between the superionic sodiums
and is consistent with low Haven's ratios in the β -alumina.

Kazuo Tsumuraya
Meiji University, Kanagawa Japan

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