

# A Hybrid-DFT Study on Sodium Ion Conductive Mechanism of $\beta$ -Alumina

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In lithium ion battery, lithium ion conductor is used for the lithium ion conductive electrolyte. Previously, we investigated the lithium ion conductive mechanism of the perovskite-type titanium oxide. It was concluded that lithium ion has the ionic bonding with other atoms, by the use of our chemical bonding rule [1-2]. In addition, we designed the new lithium ion conductive perovskite with the thermally stable structure [3-4].

Recently, sodium-sulfur battery has been much expected as rechargeable battery, as same as lithium ion battery. In sodium-sulfur battery,  $\beta$ -alumina is used for the sodium ion conductive electrolyte. We have investigated the sodium ion conductive mechanism of  $\beta$ -alumina, by the use of hybrid-DFT.

## References

- [1]T. Onishi, Solid State Ionics 180, 592, 2009.
- [2]T. Onishi, Adv. Quant. Chem., submitted.
- [3]T. Onishi, Polyhedron 28, 1792, 2009.
- [4]T. Onishi, Int. J. Quant. Chem. 109, 3659, 2009.