Hybrid-DFT study on ion conductive perovskites

Taku Onishi [a), b),c)]

a)Department of Chemistry for Materials, Graduate School of Engineering, Mie University, Tsu, Mie 514-8507 Japan

b)*The Center of Ultimate Technology on nano-Electronics, Mie University, Tsu, Mie 514-8507 Japan*

c)The Centre for Theoretical and Computational Chemistry (CTCC), Department of Chemistry, University of Oslo Postbox 1033, Blindern, 0315 Oslo, Norway

Abstract

Many perovskite-type compounds are expected as the ion conductive materials. First, we talk about our calculation results of the oxide ion conductive $LaAlO_3$ perovskite [1]. In order to clarify the oxide ion conductive mechanism in $LaAlO_3$ perovskite, hybrid-DFT calculations were performed for Onishi Ionics Model ($La_2Al_4O_3$ model). It was discovered that A-site counter cation forms the chemical bonding with conductive oxide ion (O_{cond}). We concluded that the obtained potential energy curve for oxide ion conduction can be explained by two factors such as La-O_{cond} bond formation and Al-O_{cond}-Al bond breaking. We will also talk about our calculation results for the lithium ion conductive perovskite [2-3].

References

[1] T. Onishi, Int. J. Quant. Chem. 110, 2912-2917, 2010.

[2] T. Onishi, Int. J. Quant. Chem. 109, 3659-3665, 2009.

[3] T. Onishi, Solid State Ionics 180, 592-597, 2009.