CAMT Seminar

“First-Principles Studies on Ion Migration Properties in Fast Oxide Ion Conductors for Application to Solid Oxide Fuel Cells”

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(A12 棟 1 階会議室)

Development of novel fast ion conductors is a crucial issue for realizing solid oxide fuel cells (SOFCs) which can operate in low temperatures. While yttria-stabilized zirconia (YSZ) had been well-studied both by experiments and theories, exploration of other types of materials retaining high ionic conductivities in lower temperatures is still desired. Experimental studies in the recent twenty years have found some rare-earth-based oxides having higher ionic conductivities to be promising for operation below 600°C [1-4], and first-principles simulation studies on the materials have begun [5-9]. As well as doping, introduction of strain by forming a laminate of nanoscale films was found to be an effective factor for controlling ionic conduction [3,5]. We studied atomic and electronic properties on oxygen-ionic conduction of lanthanum gallate (LaGaO3)-, lanthanum germanate (La2GeO5)-, praseodymium nickelate (Pr2NiO4)- and ceria (CeO2)-based materials by first-principles calculations based on density functional theory (DFT). We analyzed effects of doping and strain on stable structures, electronic densities of states, oxygen migration paths and activation energies in order to evaluate their capabilities in application to electrolytes. We focus on minimum energy paths of oxygen migration based on nudged elastic band analysis in order to figure out ion conduction properties in low temperatures. The obtained simulation results of the activation energies showed good agreements with experiments in several aspects. By analyzing the site dependencies of vacancy formation energies and activation energies, we inferred possible factors of preventing the oxygen ion conduction. Based on the results, we practiced iterative materials design procedures that we deduced possibly more promising compositions for the oxygen ion conduction, confirmed the properties by simulation, inferred the desirable and undesirable factors, and went back to the deduction of possibly more promising compositions. In the presentation, we will propose the designed materials and predict their electronic, magnetic and ion conduction properties.

[1] T. Ishihara, H. Matsuda and Y. Takita, J. Am. Chem. Sot. 116, 3801 (1994).
[2] M. Yashima, N. Sirikanda and T. Ishihara, J. Am Chem. Soc. 132, 2385 (2010).
[3] J. Hyodo, S. Ida, J. A. Kilner and T. Ishihara, Solid State Ionics 230, 16 (2013).
[4] T. Ishihara, et al., J. Am. Chem. Soc. 123, 203 (2001).
[5] A. Kushima and B. Yildiz, J. Mater. Chem. 20, 4809 (2010).
[6] S. M. Aspera, et al., J. Phys.: Condens. Matter 24, 405504 (2012).
[7] T. P. T. Linh, et al., J. Phys.: Condens. Matter 26, 255503 (2014).
[8] M. Alaydrus, et al., J. Phys.: Condens. Matter 25, 225401 (2013); Phys. Chem. Chem. Phys. 18, 12938 (2016).
[9] T. D. K. Wungu, et al., ECS Transactions 57, 2715 (2013).

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