Heavily Sc-doped Perovskite Oxides: Materials Design Strategy for Fast Proton Conductors

Junji Hyodo
Center for Energy System Design (CESD), International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University
hyodo.junji.524@m.kyushu-u.ac.jp

Abstract

Proton-conducting oxides are promising solid electrolyte materials for the intermediate-temperature-operable proton-conducting ceramics fuel cells (PCFCs) ranging from 300-450 ºC. The operation at such temperatures allows one to use non-heat-resistant material, reducing the manufacturing cost. However, there are no electrolyte materials attaining the commercialization requirement, conductivity exceeding 0.01 Scm^{-1} with high chemical stability, which prevents the development of intermediate-temperature operable PCFCs.

In this seminar, I present the state-of-the-art discovery of proton-conducting electrolyte solids possessing the proton conductivity of 0.01 Scm^{-1} at 300 ºC with a strategy of heavily Sc-doped perovskite oxides [1]. Coworkers and I find that $BaTiO_3$ and $BaSnO_3$ with Sc-doping to the solubility limit (70 and 80 at%, respectively) exhibit high proton conductivity. The latter material can be proved to have a high tolerance against CO_2 and worked as the electrolyte as it gained an open circuit voltage of 1.194 V at 300 ºC. These are indications that the discovered material is a potential candidate for utilization as the electrolyte for intermediate-temperature-operable PCFCs.

Further, I will discuss the role of heavy doping of Sc into perovskite from the viewpoint of local structures surrounding Sc obtained by ab initio calculations. The key feature of Sc in perovskite is likely to reduce the hopping barrier by accepting the off-center in the Sc position when the mobile protons are in the transition state. This implication would bring the design principles for the next materials discovery without expensive Sc.

[1] K. Tsujikawa, J. Hyodo, S. Fujii, K. Takahashi, S. Kasamatsu, Y. Yamazaki, "Overcoming the H^+ concentration-conductivity trade-off with heavily Sc-doped soft perovskite oxides", 21 November 2023, Preprint (Version 2) available at Research Square [https://doi.org/10.21203/rs.3.rs-3392287/v2]