# Unveiling distribution of protons and oxygen vacancies in perovskite-type proton conductors

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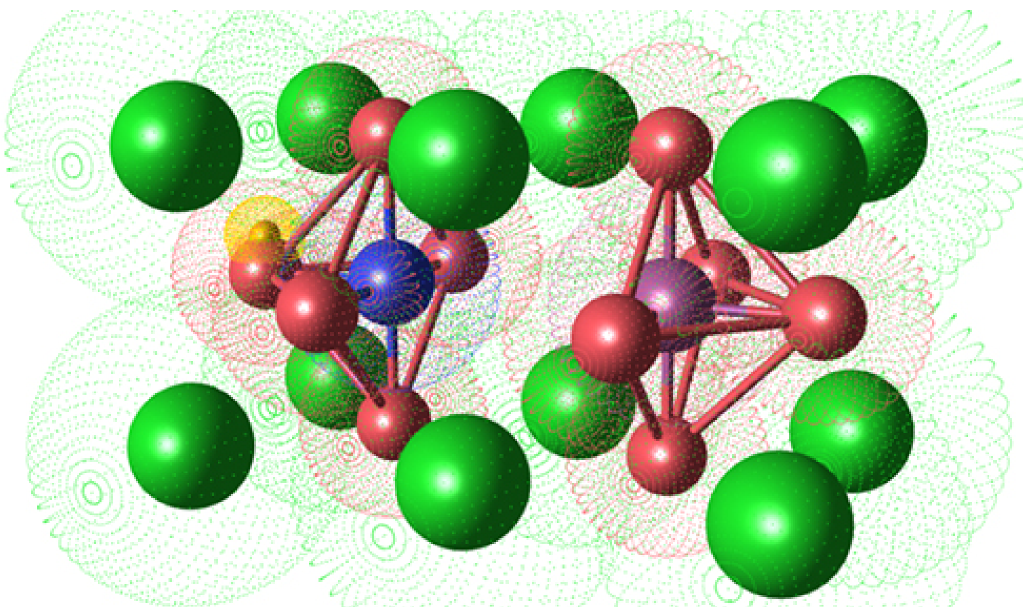


Credit: Tohoku University

Solid oxide fuel cells (SOFC), recently used as a power source for households in Japan, have several drawbacks such as high-cost, material degradation and long start-up time derived from high operating temperatures up to 750°C.

Lowering the operating temperature to an "intermediate" range of

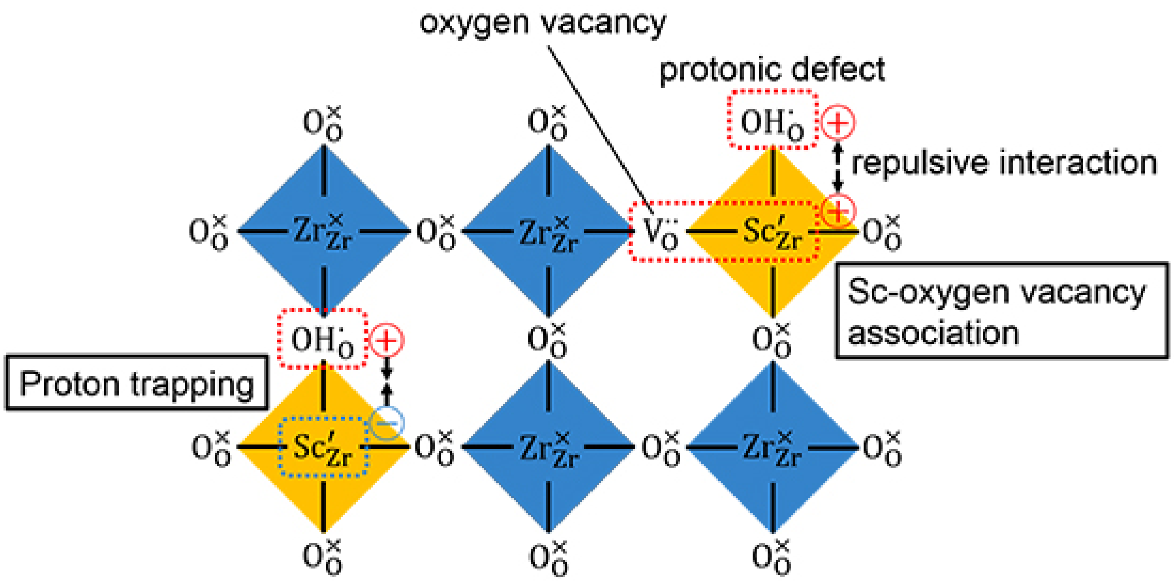
300-500°C would, in effect, enable the use of low-cost materials and allow for a quicker start-up which, in turn, could lead to wider commercial use and application to a mobile power source.

A team of researchers at Tohoku University in Japan has developed a new idea to improve proton conductivity in rare-earth doped $BaZrO_3$ perovskite-type proton conductors. Rare-earth doped $BaZrO_3$ is a promising candidate material for intermediate temperature SOFCs. However, further improvement of proton conductivity is required for practical use.

In the journal *Chemistry of Materials*, from ACS publications, the researchers suggest a strategy to improve the mobility of protons by controlling oxygen vacancies as well as protons. Protons are known to be "trapped" around a rare-earth element in the doped $BaZrO_3$ which lowers the proton conductivity. This proton trapping is originated from the electrostatic attractive interaction between a negatively charged rare-earth element and a positively charged proton.

However, when the pairing of a rare-earth element and an oxygen vacancy is created in the material, this pair possesses a positive net charge and therefore, inhibits the trapping of protons due to the electrostatic repulsive interaction.

In developing this idea, the team clarified the distribution of protons and oxygen vacancies in Sc-doped $BaZrO_3$ by combining nuclear magnetic resonance spectroscopy and thermogravimetric analysis. When a certain amount of oxygen vacancies (4 mol%) exists in the material, the proton concentration around Zr is higher than that around the rare-earth element which indicates protons with less influence from the trapping effects of the rare-earth element (Fig. 1).




(Fig. 1) Schematic view of the distribution of protons and oxygen vacancies in perovskite-type proton conductors. Credit: Tohoku University

"Because the attractive interaction between the rare-earth element and protons causes the proton trapping, introducing another defect having positive charges - that is to say, oxygen vacancy - appears to liberate the trapped protons," said Hitoshi Takamura, who led the research at Tohoku University. He and his colleagues have clarified that the interaction between the rare-earth element and oxygen vacancy does prevent the proton trapping.

"This idea can be applied not only to the development of ionic conductors but also other materials, such as fluorescent and catalyst materials, since the interaction of defects plays an important role in these materials," said Takamura. "If the distribution of defects becomes controllable, we can design a variety of functional materials. That is our goal for this research."

**More information:** Correlation among Oxygen Vacancies, Protonic

Defects, and the Acceptor Dopant in Sc-Doped $BaZrO_3$ Studied by $^{45}Sc$ Nuclear Magnetic Resonance *Chemistry of Materials* pubs.acs.org/doi/abs/10.1021/acs.chemmater.5b02441

Provided by Tohoku University