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ABSTRACT:

Nanoscale Percolation in Doped BaZrO3 for High Proton Mobility – Prediction and Experimental Results

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Yttrium-doped BaZrO3 (BZO) is known for its high proton conductivity, making it an advanced energy material for various applications, like electrolysers, fuel cells, or methane conversion cells. In our theoretical study on proton conduction in Y-doped BZO [1], density functional theory (DFT) and kinetic Monte Carlo simulations (KMC) showed that with increasing dopant fraction the proton mobility first decreases and then – after passing through a minimum – increases again. The initial decrease in mobility can be explained by trapping of protons by Y-dopants. At very low dopant fractions where it is still possible to identify isolated dopant-proton pairs, the degree of trapping is very small. With increasing dopant fraction, the equilibrium between trapped and untrapped protons shifts towards trapped protons and the fraction of free protons decreases. As a result, the average proton mobility decreases. This behaviour is well known since 1888 as Ostwald's dilution law. The following increase in mobility has, however, a different origin, namely percolation. Once the trapping zones around each dopant start to overlap, nanoscale percolation pathways start to form. If the migration barriers inside of the trapping zones are lower than outside, the result is a strong increase of the proton mobility and consequently of the proton conductivity.
Here we present our experimental results on the proton conductivity of Y-doped BZO. As a typical sign of the transition from trapping by isolated Y-ions to nanoscale percolation, the experimental results for the bulk proton mobility show a minimum as function of the Y-fraction, as predicted before by our simulations [1]. In addition, the experimental activation energy of the conductivity as a function of the Y-fraction shows good agreement with the simulations. We will also compare our predicted proton conductivities for other dopants to experimental results from literature. Finally, we will discuss a simple descriptor for the appearance of nanoscale percolation [2]. This new descriptor allows an easy screening of various dopants.

[1] F.M. Draber, C. Ader, J.P. Arnold, S. Eisele, S. Grieshammer, S. Yamaguchi, M. Martin, Nature Mater. 19, 338 (2020).

[2] F.M. Draber, J.R. Denninger, P.C. Müller, I.K. Sommerfeld, M. Martin, Adv. Energy Sustainability Res. (2022) 2200007.