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ABSTRACT:

Percolation Conduction in 3d Transition Metal Mixed Conducting Perovskite

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The mixed ionic electronic conductors of the perovskite structure ABO3 offer tuning of the electrochemical properties through its versatile range of compositions at the A-(typically alkaline earth metals) and B-sites. The bonding environment of the BO6 building blocks, where B is typically a 3d transition metal (TM), has shown to be crucial for the transport of both electronic and ionic charge carriers which is utilized in electrochemical devices such as fuel cell electrodes[1] and oxygen separation membranes (OSM). We found that substituting the B-site of the exceptionally stable but electrochemically inactive early 3d TM perovskite (SrTiO3) with the late 3d TM Co did not only yield an OSM of acceptable performance, but also enabled us to rationally identify the substitution level at which an ideal compromise of stability and activity is achieved[2]. By using the capability of X-Ray absorption spectroscopy to elucidate the element specific bonding environment, we found that a percolating network of CoO6-octahedra is necessary to facilitate conduction along the Co-O bonds, while charge carriers are trapped in isolated CoO6 manifolds below the percolation limit. These insights potentially open strategies for creating monolithic percolation materials, where different functionalities are separated in a single-phase material.

[1] Mueller, D. N., Machala, M. L., Bluhm, H. & Chueh, W. C., Nat. Commun. 6, 6097 (2015).
[2] Liu, Y., Baumann, S., Schulze-Küppers, F., Mueller, D. N. & Guillon, O., J. Eur. Ceram. Soc. 38, 5058–5066 (2018).