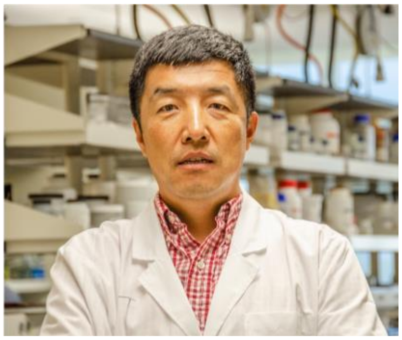

# Defects, Mixed Ionic-Electronic Conductors, and in Solid Oxide Electrochemical Cells

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Dr. Xingbo Liu received his Ph.D. on Materials Science from University of Science and Technology Beijing in 1999, and he subsequently went to West Virginia University as a postdoc. Currently, he is the Interim Associate Dean of Research and Statler Endowed Chair Professor in Statler College of Engineering and Mineral Resources at West Virginia University. Dr, Liu's has developed an international recognized research program on materials for next generation energy conversion and storage, with the focus on high temperature materials such as solid oxide fuel cells & high temperature Ni-Superalloys. Dr. Liu has received numerous awards, including one R&D 100 Award (2011) for his development of SOFC interconnect coating, TMS Early Career Faculty Fellow Award (2010), TMS Brimacombe Medal (2016), State of West Virginia Innovator of the Year (2013), WVU CEMR Researcher of the Year (2015, 2011), Outstanding Researcher Awards (2015, 2011, 2009, 2008), and several others. He is the Fellow of ASM International and American Ceramics Society.

## Abstract

Solid Oxide Electrochemical Cells (SOCs) are promising electrochemical devices in clean energy conversion and storage. Key to improve the efficiency and reaction kinetics of SoCs is to control the defect chemistry in mixed ionic-electronic conducting (MIEC) electrodes. We developed a multi-domain physical model incorporating multi-step charge transfer to examine the competitive behaviors between the paralleled triple phase boundary (3PB) and two-phase boundary (2PB) kinetic pathways. Analyses identified the limitation of surface oxygen ion diffusion as the mechanism for 3PB-to-2PB transition. The model also proved surface reactions are driven predominantly by electrochemical forces at the 3PB, while being controlled by oxygen vacancy concentration variation at regions away from 3PB. Then, we investigated the long-term performance degradation of LSM/YSZ composite cathodes via calibrated multi-physics simulation with the multistep ORR model and structural coarsening data from a phase field study. The multi-physics model is simultaneously calibrated with experimental polarization curves and impedance behavior for various air/fuel supply conditions. The calibrated simulations are utilized to simulate a 2D half-cell constructed with measured microstructural data and random heterogeneity. The long-term performance degradation of the half-cell is predicted by the calibrated multi-physics model coupled with structural coarsening trends simulated using a phase field-based coarsening model. Degradation of both polarization curves and impedance behavior is investigated. Thorough analyses, including changes of contributions from different pathways, the resistance components, and overall reaction order, are performed to provide more insights into cathode performance degradation due to grain coarsening phenomena.