22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

Materials Discovery Through Interpretation: Intermediate-Temperature Protonic Ceramic Fuel Cells

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Key Words: proton, oxide, machine learning, protonic ceramic fuel cells.

Materials Discovery through Interpretation (MDI) integrates scientific reasoning into machine-learning (ML) workflows to enable reliable extrapolation beyond training data [1-2]. We demonstrate this approach for proton-conducting oxides and its translation into a protonic ceramic fuel cell (PCFC) operating below 350 °C. ML screening first identified rhombohedral SrSn0.8Sc0.2O3-δ as a candidate proton conductor [3]. Based on prior findings [2,4], we replaced Sr with Ba to obtain the cubic perovskite structure and increased the Sc content from 20 to 70 at.%. The resulting BaSn0.3Sc0.7O3-δ achieves a proton conductivity of 0.01 S cm-1 at 300 °C, where proton diffusion along ScO_6 octahedral networks mitigates proton trapping [5]. Extending this strategy to BaTi0.2Sc0.8O3-δ (BTS80) yielded an even higher conductivity of 0.016 S cm-1. We fabricated the first PCFC with a pulsed-laser-deposited BTS80 thin-film electrolyte on a Pd anode and a triple-conducting PrBa0.5Sr0.5Co1.5Fe0.5O5+δ cathode, achieving 146 and 233 mW cm-2 at 300 and 350 °C, respectively. Detailed electrochemical and microstructural analyses of the PCFC, including impedance spectroscopy and high-resolution transmission electron microscopy, will be presented to identify the dominant loss mechanisms and guide future materials and interface design for sub-350 °C operation.

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