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ABSTRACT:

Computational and Experimental Approach to High-Performance BaHfO₃-Based Electrolytes for Proton Conduction Electrochemical Cells

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Proton-conducting electrochemical cells (PCECs) have emerged as a promising technology for efficient energy conversion and storage. However, the development of stable and highly conductive electrolyte materials remains a critical challenge. In this study, we investigate BaHfO₃-based perovskite oxides as potential candidates for next-generation PCEC electrolytes. We employ a synergistic approach combining density functional theory (DFT) calculations and experimental validation to elucidate the proton transport mechanisms and electrochemical performance of Yttrium-doped BaHfO₃ (BaHf_{0.8}Y_{0.2}O₃). DFT calculations demonstrate that Y-doping effectively introduces oxygen vacancies and facilitates proton incorporation, leading to a favorable proton migration energy landscape within the BaHfO₃ lattice. Complementary experimental characterization, including X-ray diffraction, scanning electron microscopy, and electrochemical impedance spectroscopy (EIS), confirms that the synthesized BaHfO₃ phase exhibits excellent proton conductivity and chemical stability under operating conditions. Our findings indicate that Y-doped BaHfO₃ demonstrates superior ionic transport characteristics compared to traditional perovskite systems. This study highlights the potential of BaHfO₃ as a robust and high-performance electrolyte material, providing a clear pathway for the design and optimization of advanced proton-conducting ceramics for electrochemical applications.