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ABSTRACT

Accelerated Proton Transport Via ScO_6 Octahedral Networks in Cubic Perovskite Oxides with High Sc Content

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Efficient proton transport in solid-state electrolytes is crucial for achieving high-performance proton ceramic fuel cells and electrolysers [1-4], yet proton trapping at acceptor dopant sites severely limits ionic conductivity [5]. Here, we demonstrate that high scandium (Sc) content in cubic perovskite oxides significantly accelerates proton transport through the formation of interconnected ScO_6 octahedral networks. Specifically, BaSc0.7Sn0.3O3-□ exhibits proton conductivity exceeding the technological benchmark of 0.01 Scm-1 at 300°C [6], effectively overcoming traditional conductivity trade-offs. Molecular dynamics simulations utilizing machine-learning force fields confirm that Sc-rich octahedral networks facilitate continuous and rapid proton diffusion, substantially reducing proton trapping. These results provide guidelines for optimizing proton conduction in perovskite oxides and introduce a promising strategy to design stable electrolytes with enhanced proton diffusivity at intermediate operating temperatures.

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