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ABSTRACT

Modeling and Validation of Phase Stability of Ceria-Zirconia Solid Solutions under Diverse Thermodynamic Conditions

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Over the past decades, CeO_2-ZrO_2 solid solutions (CZO) have emerged as a superior alternative to conventional CeO_2 as catalyst support materials in three-way catalysts (TWCs) due to their enhanced oxygen storage capacity (OSC). CeO_2-rich CZO compositions, in particular, exhibit the highest OSC. However, the phase stability of CeO_2-rich CZO remains controversial, as numerous studies report conflicting observations regarding its structural and compositional stability. Recent experimental findings have further intensified this debate, revealing for the first time that CeO_2-rich CZO can completely phase-separate into CeO_2 and ZrO_2 under typical catalyst operating conditions. To address this issue, this study explores alternative CZO compositions with improved stability under standard catalytic and electrochemical device conditions, including solid oxide fuel cells (SOFCs). Thermodynamic calculations and defect chemical analysis were conducted to evaluate the stability of various CZO compositions, followed by experimental validation of their calculated results. These findings provide new insights into the design and application of stable CZO-based materials for catalytic and electrocatalytic applications.