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Defect-Engineered Ceria-Supported Ru Catalysts for Enhanced Ammonia to Hydrogen Conversion.

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ABSTRACT

Ammonia decomposition presents a critical pathway for hydrogen production and storage by enabling ammonia as a carbon-free hydrogen carrier; however, catalyst deactivation and inefficient nitrogen activation remain key challenges. Herein, we report a defect-engineered ceria-supported ruthenium catalyst, developed by integrating atomic-scale dispersion of Ru with controlled lattice modification of the support. Ruthenium is stabilised as isolated atoms and sub-nanometre clusters on a praseodymium–cobalt co-doped ceria matrix synthesised via an optimised sol gel route, maximising accessible active sites while suppressing sintering. The incorporation of aliovalent co-dopants into a ceria matrix leads to a significant increase in oxygen vacancy concentration and electronic structure, resulting in modified metal–support interactions and enhanced redox capability. These materials' level modifications facilitate N-H bond activation, leading to near-complete ammonia conversion under the investigated conditions. The optimised RC-$Pr_{0.3}Co_{0.2}O_x$ catalyst outperforms undoped ceria and benchmark 1 wt% Ru–CeO_2 in both activity and long-term stability. The results highlight defect-mediated metal–support synergy as an interdisciplinary materials design strategy for advancing ammonia cracking catalysts toward integration in solid oxide fuel cell–based, carbon-neutral energy systems.

KEY WORDS

Hydrogen Production, Ammonia Cracking, Single-atom catalysts, Defect Engineering.

BIOGRAPHY

Pallavi Saini is a Ph.D. researcher in Applied Chemistry specializing in carbon capture, nanomaterials, and ammonia cracking, with a focus on advancing cleaner energy and sustainable solutions. Skilled in material synthesis, advanced characterization, and catalysis, she combines technical expertise with a passion for turning research into real-world impact. Beyond the lab, she is a dedicated science communicator who thrives on collaboration, mentorship, and meaningful dialogue that connects research to the communities it serves.

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