Supplementary Information (SI) for Journal of Materials Chemistry A.

Supporting Information

Enhancing ammonia decomposition in a $LaCeO_x$/Ni inverse catalyst by tuning lattice strain and oxygen vacancies

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Considering economic and performance factors, Ni is the preferred non-noble metal catalyst for ammonia decomposition. Therefore, various inverse Ni-based catalysts were synthesized using the stepwise precipitation method. As shown in Fig. S1a, at 550 °C, although the ammonia conversion rate of $LaCeO_x/Ni$ was slightly lower than that of $LaCeO_x/Ni_{40}$ and $LaCeO_x/Ni_{60}$, all three achieved over 90% conversion (60000 mL $(g_{cat}\ h)^{-1}$), indicating that increasing Ni loading beyond 30% has limited effect on performance improvement. Nevertheless, both the ammonia conversion and hydrogen production rate of $LaCeO_x/Ni$ were significantly enhanced by approximately 6% and 4 mmol $(g_{cat}\ min)^{-1}$, respectively, compared to $LaCeO_x/Ni_{20}$ (Fig. S1b). Therefore, $LaCeO_x/Ni$ was selected as the optimal balance among activity, economic viability, and stability. Moreover, as shown in Fig. S1c−d, $LaCeO_x/Ni$ exhibited notably superior catalytic performance compared to $La_3Ce_7O_x/Ni$ and $La_7Ce_3O_x/Ni$, demonstrating that $LaCeO_x$ is the optimal support when the Ni loading reaches 30%. In summary, $LaCeO_x/Ni$ was confirmed as the optimal combination of metal loading and support composition within this catalyst system, demonstrating excellent and balanced high activity across the temperature range of 350−600 °C, indicating significant practical feasibility.

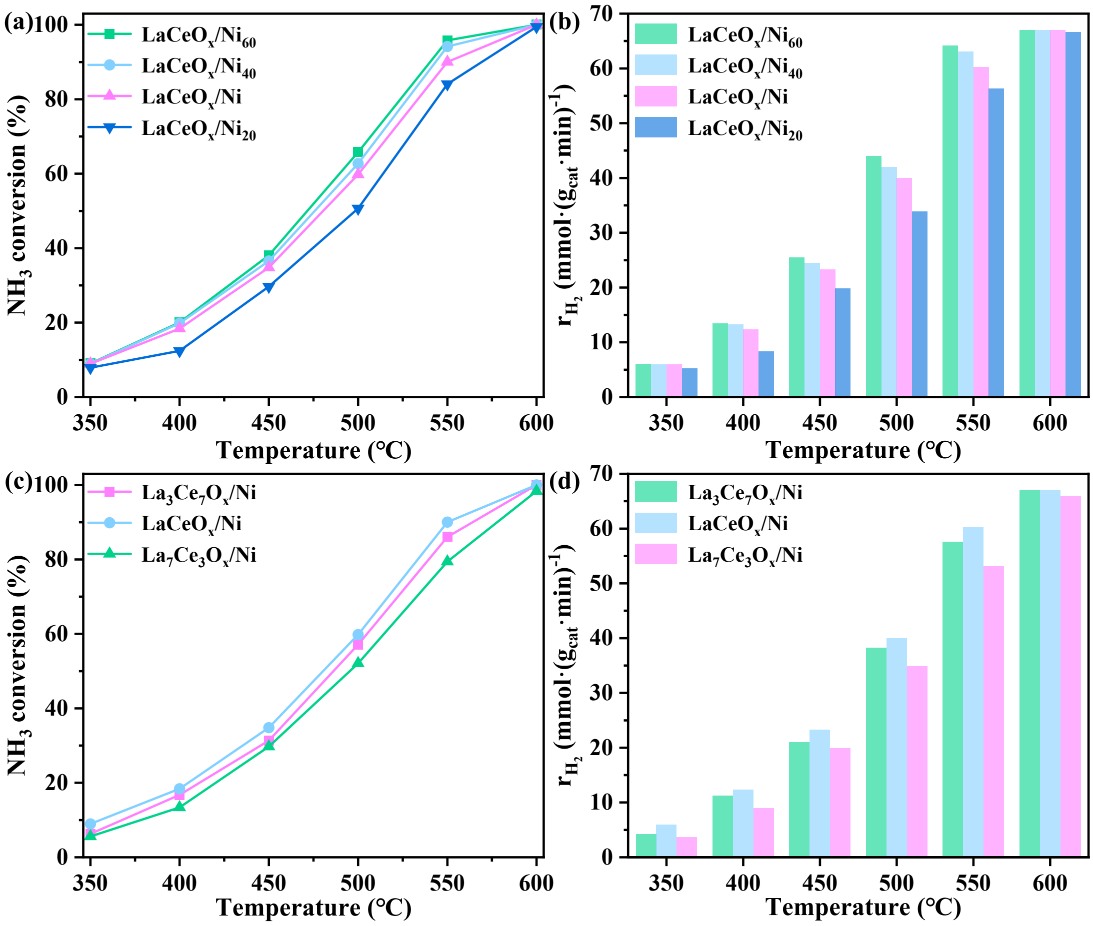

Fig. S1 Temperature–dependent activities of the LaCeO$_x$/Ni catalysts. (a) Different Ni content in LaCeO$_x$/Ni catalysts (b) Different La content in LaCeO$_x$/Ni catalysts. GHSV = 60000 mL (g$_{cat}$ h)$^{-1}$

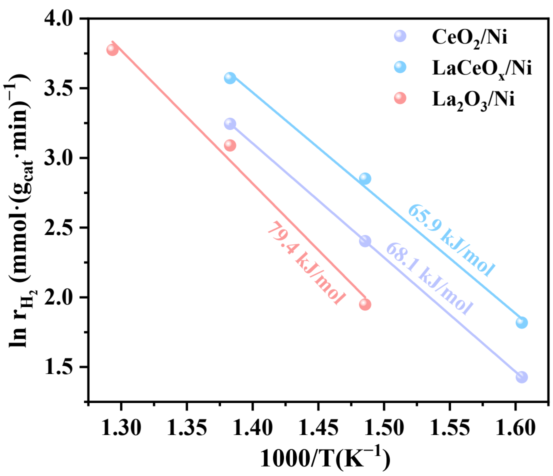

Fig. S2 Arrhenius plots of CeO$_2$/Ni, LaCeO$_x$/Ni, and La$_2$O$_3$/Ni.

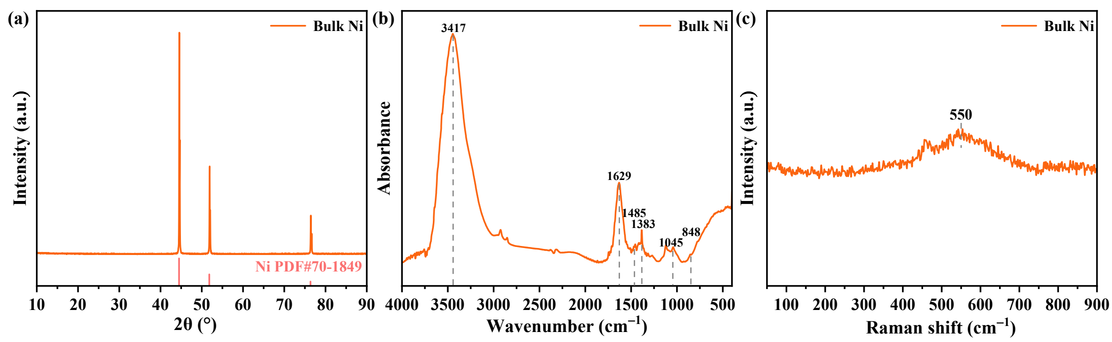

Fig. S3 (a) XRD pattern, (b) FTIR spectra, (c) and Raman spectra of the Bulk Ni.

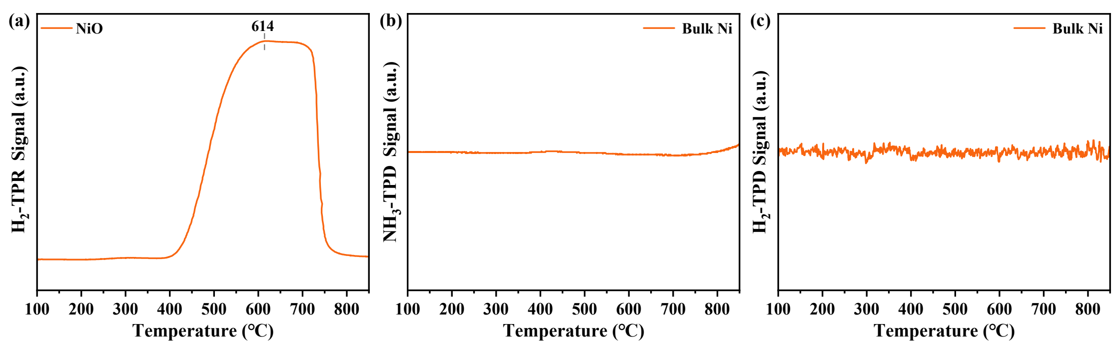

Fig. S4 (a) H_2-TPR of the NiO; (b) NH_3-TPD and (c) H_2-TPD profiles of the Bulk Ni.

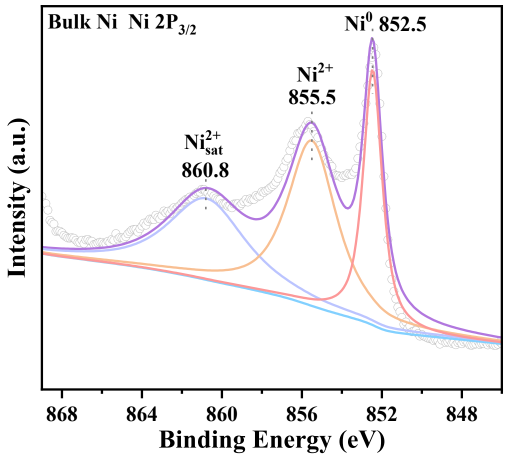

Fig. S5 Ni $2p_{3/2}$ XPS spectra of the Bulk Ni catalysts.

Table S1 XPS, and ICP parameters of the Bulk Ni catalyst.

Catalysts	Ni (wt%)	Ni^0/Ni^{2+}
Bulk Ni	67.3	0.487