International Journal of Trend in Scientific Research and Development (IJTSRD)
Volume 10 Issue 5, Sep-Oct 2026 Available Online: www.ijtsrd.com e-ISSN: 2456 – 6470

Structure–Surface Relationships and Catalytic Behaviour of Rare-Earth Transition-Metal Perovskites: A Comparative Analysis of Oxygen Mobility, Acidity and Redox Behaviour

Jyoti Kumari[1], Rabindra Kumar[2], Vijay Kumar[3], Sima Kumari[4]

[1,3,4]Research Scholar, [2]Associate Professor,
[1,2,3]University Department of Chemistry, T.M. Bhagalpur University, Bhagalpur, Bihar, India
[4]Bhagalpur College of Engineering, Sabour, Bhagalpur, Bihar, India

ABSTRACT

Rare-earth transition-metal perovskites with the general formula $LnMO_3$ constitute an important class of mixed-metal oxides with considerable potential in heterogeneous catalysis. Their catalytic behaviour is closely associated with the nature of the B-site transition metal, oxygen mobility, oxygen-vacancy concentration, surface acidity and the redox flexibility of the lattice. The present study provides a comparative analysis of selected $LnMO_3$ systems using reported data for $LaMnO_3$, $LaFeO_3$, $LaCoO_3$, $LaNiO_3$, $LaCo_{0.8}Mn_{0.2}O_3$, $YCoO_3$ and $YNiO_3$. Particular attention is given to the relationship between calcination temperature and surface properties of $YCoO_3$ and $YNiO_3$, together with their catalytic behaviour during thermal decomposition of urea. The available data indicate that increasing calcination temperature produces a progressive decrease in excess surface oxygen and surface acidity. $YNiO_3$ exhibits comparatively higher surface acidity than $YCoO_3$, while its reported lower activation energy during urea decomposition indicates favourable catalytic kinetics. Comparison of different B-site compositions further indicates that mixed Co–Mn perovskites can benefit from synergistic redox interactions and enhanced oxygen-vacancy formation. The analysis demonstrates that catalytic performance in $LnMO_3$ materials cannot be attributed to a single structural parameter but arises from the combined influence of composition, surface oxygen, acidity, oxygen mobility and redox characteristics.

KEYWORDS: *$LnMO_3$, perovskite oxide, mixed transition-metal oxide, oxygen vacancy, surface acidity, oxygen mobility, $YCoO_3$, $YNiO_3$, heterogeneous catalysis.*

How to cite this paper: Jyoti Kumari | Rabindra Kumar | Vijay Kumar | Sima Kumari "Structure–Surface Relationships and Catalytic Behaviour of Rare-Earth Transition-Metal Perovskites: A Comparative Analysis of Oxygen Mobility, Acidity and Redox Behaviour" Published in International Journal of Trend in Scientific Research and Development (ijtsrd), ISSN: 2456-6470, Volume-10 | Issue-5, October 2026, pp.854-860, URL: www.ijtsrd.com/papers/ijtsrd142164.pdf

IJTSRD142164

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1. INTRODUCTION

Mixed transition-metal oxides have attracted considerable attention as heterogeneous catalysts because their crystal structures can accommodate different metal ions while maintaining substantial thermal and chemical stability. Among these materials, perovskite-type oxides represented by the general formula $LnMO_3$ provide considerable flexibility for modifying catalytic properties through substitution at the A- and B-sites.

In a typical $LnMO_3$ structure, the lanthanide ion occupies the A-site and a transition-metal ion occupies the B-site. The B-site metal is particularly important because it participates directly in redox processes and influences metal–oxygen bonding, oxygen mobility and surface reaction pathways. Previous studies have therefore associated the catalytic performance of these oxides with transition-metal composition, lattice oxygen and oxygen vacancies.

The available information on La- and Y-based perovskites provides an opportunity to examine catalytic behaviour from a structure–surface perspective rather than simply comparing individual catalysts. The present analysis therefore combines

representative catalytic systems with reported surface-property and kinetic observations for $YCoO_3$ and $YNiO_3$.

The source data indicate that oxygen vacancies can promote adsorption and surface reactions, while changes in calcination temperature modify excess surface oxygen and acidity.

2. Objective of the Study

The objective of the present work is to develop a comparative interpretation of selected $LnMO_3$ perovskites by examining:

1. the influence of B-site transition-metal composition on catalytic behaviour;
2. the relationship between calcination temperature and surface oxygen;
3. the relationship between calcination temperature and surface acidity;
4. the comparative behaviour of $YCoO_3$ and $YNiO_3$ during urea decomposition; and
5. the possible contribution of oxygen vacancies and mixed B-site composition to catalytic performance.

The study is based on secondary analysis of the information and data presented in the supplied published papers. It does not claim the reported measurements as newly performed experiments.

3. Structural Characteristics of $LnMO_3$ Perovskites

The basic perovskite structure can be represented as $LnMO_3$, where Ln denotes a rare-earth element and M represents a transition metal. The A-site ion is generally larger and is surrounded by oxygen atoms, whereas the smaller B-site transition metal is situated within an oxygen octahedral environment.

The structural flexibility of these materials permits variation in both cationic positions. Such variation can modify lattice distortion, metal–oxygen bonding, oxygen-vacancy concentration and the oxidation states of transition metals. Consequently, apparently similar perovskite structures may display substantially different catalytic behaviour.

The principal catalytic features associated with $LnMO_3$ materials include oxygen vacancies, mixed oxidation states, oxygen mobility and strong metal–oxygen interactions.

4. Comparative Catalytic Behaviour of Selected $LnMO_3$ Systems

The reported catalytic systems demonstrate that changing the B-site transition metal changes the dominant catalytic application.

Table 1. Comparative catalytic characteristics of selected $LnMO_3$ perovskites

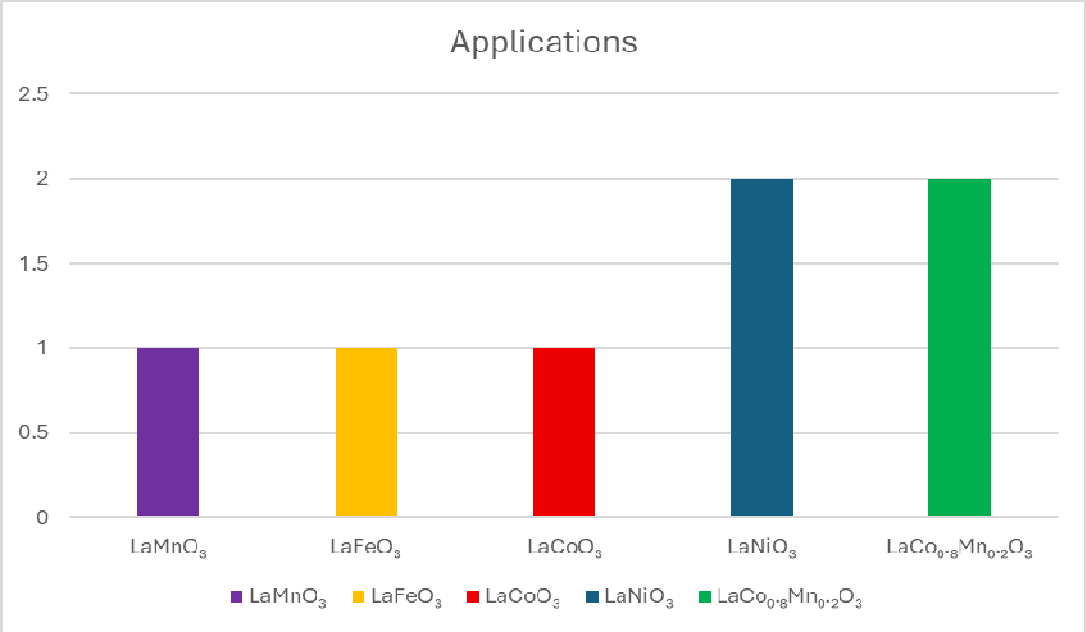
Perovskite	B-site metal	Reported catalytic application	Principal catalytic characteristic
$LaMnO_3$	Mn	Oxygen reduction reaction (ORR)	Redox-active Mn centre
$LaFeO_3$	Fe	Hydrocarbon oxidation	Oxygen-mediated oxidation
$LaCoO_3$	Co	CO oxidation	Redox-active Co–O surface
$LaNiO_3$	Ni	CO and benzene oxidation	Reactive lattice oxygen and redox flexibility
$LaCo_{0.8}Mn_{0.2}O_3$	Co–Mn	CO and NO oxidation	Synergistic Co–Mn interaction and oxygen-vacancy formation

The comparative information indicates that $LaNiO_3$ shows high activity for CO oxidation, while $LaCoO_3$ shows moderate activity for the same reaction. $LaMnO_3$ is associated with high activity in oxygen reduction, whereas $LaCo_{0.8}Mn_{0.2}O_3$ is reported to exhibit very high activity toward CO/NO oxidation.

These differences demonstrate the importance of B-site composition. Rather than treating all perovskites as equivalent catalysts, the transition-metal centre should be considered a major determinant of surface redox chemistry.

Reported Catalytic Applications of Selected $LnMO_3$ Perovskites

Number of distinct catalytic applications reported for each perovskite in the comparative table.



Graph1: Application count is descriptive only and does not represent catalytic activity or conversion efficiency.

5. Effect of Calcination Temperature on Surface Properties

One of the most useful datasets in the supplied material concerns $YCoO_3$ and $YNiO_3$. The samples are designated YC1–YC4 and YN1–YN4, respectively. The reported graphical data examine excess surface oxygen and surface acidity at different calcination temperatures.

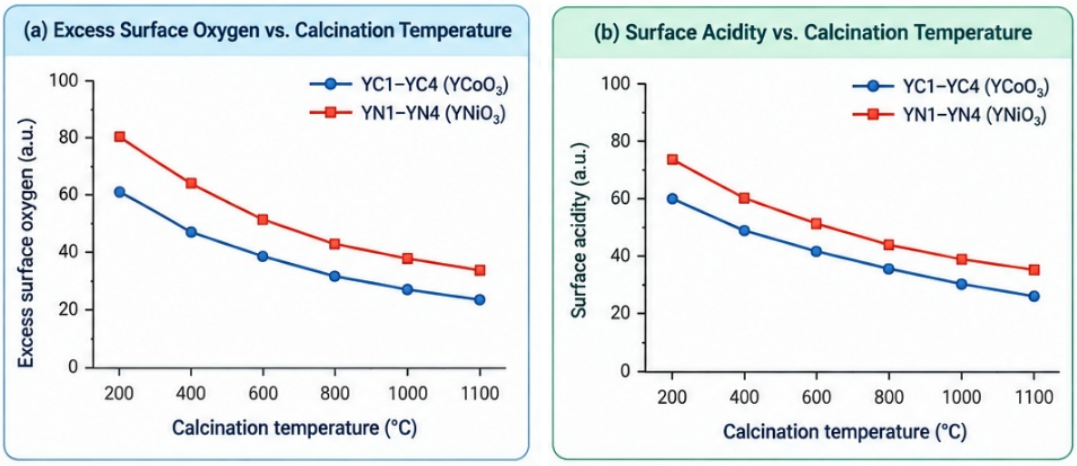
The source graph covers calcination temperatures extending approximately from 200 to 1100 °C. The important observation is not simply the absolute temperature but the systematic change in surface properties with thermal treatment.

Table 2. Source-reported surface-property trends for $YCoO_3$ and $YNiO_3$

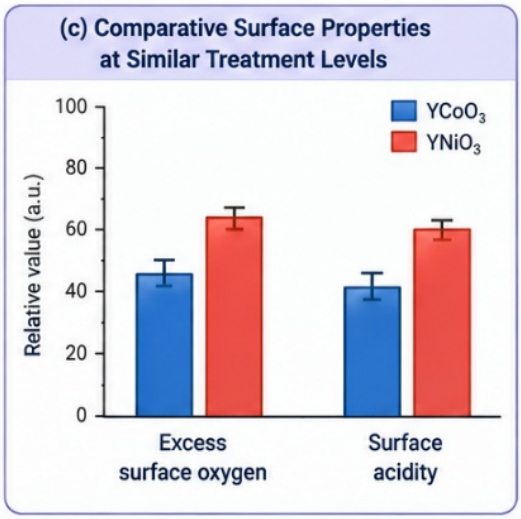
Sample series	Calcination treatment	Excess surface oxygen	Surface acidity	Overall trend
YC1–YC4	Increasing temperature	Progressive decrease	Progressive decrease	Surface oxygen and acidity decline with thermal treatment
YN1–YN4	Increasing temperature	Progressive decrease	Progressive decrease	Surface oxygen and acidity decline; acidity remains comparatively higher than $YCoO_3$
$YCoO_3$ vs $YNiO_3$	Comparable treatment levels	Temperature dependent	$YNiO_3$ comparatively higher	Different B-site metals produce different surface characteristics

The supplied data specifically report a gradual reduction in excess surface oxygen and surface acidity with increasing calcination temperature. $YNiO_3$ samples exhibited comparatively higher acidity, suggesting that the identity of the transition metal modifies the surface response to thermal treatment.

It is important to note that the original source presents these values primarily through graphical representations. Therefore, exact numerical values should not be reconstructed from the graph unless the authors' original numerical dataset is available. The present table consequently reports the experimentally indicated trends rather than introducing estimated numbers.



A B



C

Graphical Representation (A,B & C) of Temperature on Surface Oxygen and acidity of $YCoO_3$ and $YNIO_3$

6. Surface Oxygen and Oxygen-Vacancy Chemistry

Surface oxygen plays an important role in oxidation catalysis. During catalytic operation, lattice or surface oxygen can participate directly in the oxidation of adsorbed reactants. Removal of oxygen from the lattice can generate oxygen vacancies, which may subsequently be replenished by gaseous oxygen.

The supplied study associates increased oxygen-vacancy availability with enhanced catalytic performance and improved adsorption and surface reaction processes.

This observation provides a useful interpretation of the $YCoO_3$ and $YNiO_3$ results. Calcination changes the surface environment, and the decrease in excess surface oxygen with increasing temperature suggests that thermal treatment alters the number or nature of catalytically accessible oxygen species (Zhang, et al, 2027).

However, an excessive reduction in surface oxygen should not automatically be interpreted as improved catalytic performance. Catalysis requires a balance between oxygen removal and oxygen replenishment. A catalyst must therefore possess sufficient oxygen mobility to participate in a complete redox cycle.

7. Surface Acidity as a Catalytic Parameter

Surface acidity provides another important dimension for understanding the catalytic behaviour of perovskite oxides. The reported $YCoO_3$ and $YNiO_3$ data demonstrate that the two materials do not possess identical acidic characteristics.

$YNiO_3$ exhibits comparatively higher surface acidity than $YCoO_3$ under the investigated conditions. This distinction may influence adsorption and activation of reactant molecules and may partly contribute to the different catalytic behaviour observed for the two materials (Zhu, 2015).

The reduction in acidity with increasing calcination temperature also suggests that thermal treatment can alter the concentration or accessibility of catalytically active surface sites. Thus, calcination should be considered not merely a preparation step but a factor capable of modifying the catalytic surface.

8. Comparative Analysis of Urea Decomposition

The second major dataset concerns the thermal decomposition of urea in the presence of $YCoO_3$ and $YNiO_3$ catalysts. The source compares an uncatalysed urea system with YC1–YC4 and YN1–YN4 catalyst samples sites (Liu, et al, 2021).

The reported kinetic comparison considers rate constants at **140°C, 150°C and 160°C**, together with activation energy. The graphical presentation indicates that both $YCoO_3$ and $YNiO_3$ substantially increase the rate of urea decomposition relative to the uncatalysed reaction.

Table 3. Comparative kinetic information reported for urea decomposition

System	Rate measurements reported at	Activation-energy comparison	Reported interpretation
Urea without catalyst	140, 150 and 160°C	Reference system	Lowest catalytic assistance
$YCoO_3$ (YC1–YC4)	140, 150 and 160°C	Reduced relative to uncatalysed reaction	Catalytic enhancement of decomposition
$YNiO_3$ (YN1–YN4)	140, 150 and 160°C	Relatively lower activation energy	Comparatively favourable catalytic efficiency

The source reports that both $YCoO_3$ and $YNiO_3$ enhance the thermal decomposition rate of urea. It further reports that $YNiO_3$ exhibits relatively lower activation energies, indicating more favourable catalytic kinetics under the investigated conditions. Catalytic performance was also reported to depend on calcination temperature and transition-metal composition.

This result is particularly relevant because it demonstrates that surface acidity and oxygen characteristics should be interpreted together with kinetic behaviour. A catalyst possessing a particular surface property does not necessarily show enhanced activity unless that property contributes effectively to the reaction pathway.

9. Role of Mixed B-Site Composition

The catalytic properties of perovskites can also be modified by introducing more than one transition metal into the B-site. $LaCo_xMn_{1-x}O_3$ is an example of such a mixed B-site system.

The reported $LaCo_{0.8}Mn_{0.2}O_3$ composition shows very high catalytic activity toward CO and NO oxidation. Its enhanced performance has been associated with improved oxygen-vacancy formation and electron-transfer characteristics.

Table 4. Comparative interpretation of B-site composition

B-site configuration	Representative catalyst	Reported catalytic behaviour	Possible controlling feature
Single Mn	$LaMnO_3$	High ORR activity	Mn redox chemistry
Single Fe	$LaFeO_3$	Hydrocarbon oxidation	Fe–O redox interaction
Single Co	$LaCoO_3$	CO oxidation	Co redox flexibility
Single Ni	$LaNiO_3$	CO/benzene oxidation	Reactive oxygen/redox chemistry
Mixed Co–Mn	$LaCo_{0.8}Mn_{0.2}O_3$	Very high CO/NO oxidation	Synergistic redox interaction

The comparison suggests that combining transition metals can create catalytic properties that differ from those of the corresponding single-metal perovskites. Such behaviour may arise from changes in oxidation-state distribution, oxygen-vacancy formation and electron transfer.

10. Relationship Between Calcination, Surface Properties and Catalysis

The combined observations from the available data can be represented as a conceptual relationship:

Calcination temperature → surface oxygen/acidity → oxygen mobility and active-site characteristics → adsorption and reaction kinetics → catalytic performance

The $YCoO_3$/$YNiO_3$ observations demonstrate that increasing calcination temperature changes the surface properties. At the same time, the urea-decomposition data show that catalyst performance is temperature- and composition-dependent.

This indicates that an optimum catalytic surface is unlikely to be determined by one parameter alone. Excess surface oxygen, oxygen vacancies, acidity,

transition-metal oxidation states and surface structure may interact to determine the final catalytic response (Ercan et al, 2025).

11. Possible Catalytic Mechanism

The oxidation behaviour of $LnMO_3$ perovskites can be interpreted using the Mars–van Krevelen concept. In this mechanism, a reactant interacts with oxygen associated with the catalyst surface or lattice. Consumption of lattice oxygen creates an oxygen vacancy, after which the catalyst can be reoxidized by gaseous oxygen (Li, 2023).

The simplified catalytic sequence can therefore be represented as:

Reactant adsorption → reaction with lattice/surface oxygen → product formation → oxygen-vacancy generation → catalyst reoxidation

The effectiveness of this cycle depends on the ability of the catalyst to provide and subsequently replenish reactive oxygen. The reported importance of oxygen vacancies and oxygen mobility in $LnMO_3$ catalysts is consistent with this interpretation.

12. Environmental and Energy Applications

$LnMO_3$ perovskites have potential applications in environmental catalysis because their redox properties can be utilized for the conversion of pollutants. Reported applications include CO oxidation, NOx-related oxidation processes, hydrocarbon oxidation and degradation of organic pollutants.

$LaCoO_3$ has been associated with CO oxidation, $LaFeO_3$ with organic-pollutant degradation, $LaMnO_3$ with oxygen reduction, and $LaNiO_3$ with benzene oxidation.

These materials are also relevant to energy-conversion technologies, including fuel cells, water-splitting reactions and hydrogen production. Their usefulness in such applications is related to their electronic conductivity, oxygen mobility and redox flexibility.

13. Discussion

The comparative analysis reveals three major relationships.

First, **B-site composition is a fundamental determinant of catalytic behaviour**. The comparison among $LaMnO_3$, $LaFeO_3$, $LaCoO_3$ and $LaNiO_3$ shows that changing the transition-metal centre changes the principal catalytic application. This is consistent with the role of B-site ions in controlling redox behaviour and metal–oxygen interactions (Mabate et al, 2023).

Second, **thermal treatment modifies surface properties**. The $YCoO_3$ and $YNiO_3$ data demonstrate that increasing calcination temperature is accompanied by a decrease in excess surface oxygen and surface acidity. This means that preparation conditions can modify the population of catalytically relevant surface sites (Liu, et al, 2021).

Third, **surface properties and catalytic kinetics are interconnected but not identical**. $YNiO_3$ possesses comparatively higher acidity and is also reported to exhibit relatively lower activation energy during urea decomposition. However, these observations should be treated as correlations rather than proof that acidity alone determines catalytic performance (Misono, 2023).

The mixed B-site system $LaCo_{0.8}Mn_{0.2}O_3$ provides an additional indication that catalytic enhancement can result from interactions between different transition metals. Its reported high activity for CO and NO oxidation has been associated with oxygen-vacancy formation and electron transfer (Nitadori, 1988).

Taken together, the data support a multidimensional model in which **composition + oxygen chemistry + acidity + thermal history + redox flexibility** collectively determine catalytic performance.

14. Conclusion

The present comparative analysis demonstrates that rare-earth transition-metal perovskites exhibit substantial variation in catalytic behaviour depending on their B-site composition and surface characteristics. $LaMnO_3$, $LaFeO_3$, $LaCoO_3$ and $LaNiO_3$ represent distinct examples in which different transition metals are associated with different catalytic reactions.

The $YCoO_3$ and $YNiO_3$ data provide additional evidence that calcination temperature strongly affects excess surface oxygen and surface acidity. Both properties show a decreasing trend with increasing calcination temperature, while $YNiO_3$ exhibits comparatively higher acidity. The kinetic data for urea decomposition further indicate that both perovskites enhance decomposition relative to the uncatalysed system, with $YNiO_3$ showing relatively lower activation energy.

The analysis also highlights the importance of mixed B-site compositions. $LaCo_{0.8}Mn_{0.2}O_3$ demonstrates how combining transition metals can produce synergistic catalytic behaviour associated with oxygen vacancies and electron transfer.

Overall, the available data indicate that the catalytic properties of $LnMO_3$ perovskites arise from an interconnected network of structural, surface and

electronic characteristics. Future investigations should therefore consider composition, calcination conditions, oxygen mobility, surface acidity and redox behaviour simultaneously rather than treating any single parameter as an independent predictor of catalytic activity.

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International Journal of Trend in Scientific Research and Development
IJTSRD
International Journal of Trend in Scientific Research and Development
ISSN: 2456-6470