

Diseño Basado en Datos de Nanoestructuras de CeO₂ con Morfología Controlada y Propiedades Catalíticas Ajustables

Data-Driven Design of CeO₂ Nanostructures with Controlled Morphology and Tunable Catalytic Properties

B. Trujillo-Navarrete ^{a, *}

^a Centro de Graduados e Investigación en Química, Tecnológico Nacional de México, IT. de Tijuana, 22414 Tijuana, Baja California, México.

Resumen

Las nanoestructuras de óxido de cerio (CeO₂) con morfologías controladas (esferulitas, nanobarras cortas y nanobarras largas) se sintetizaron mediante un diseño factorial que varió la concentración de octadecilamina (0.01–0.2 M) y la relación etanol/agua ($\alpha = 0.3$ –3.0). A partir de una caracterización exhaustiva, se seleccionaron 15 propiedades fisicoquímicas clave para un análisis multivariante. El análisis de componentes principales reveló una agrupación morfológica: el primer componente principal (55 % de varianza) separó las muestras según la densidad de defectos y el área superficial, mientras que el segundo componente principal (25 % de varianza) lo hizo según la relación de aspecto. La regresión por Mínimos Cuadrados Parciales mostró que los parámetros de síntesis explican más del 90 % de la varianza en las propiedades, siendo la concentración de octadecilamina el factor dominante. El método de K-medias confirmó tres grupos diferenciados. La proyección uniforme de variedades y aproximación (UMAP) proporcionó una visualización no lineal superior, sugiriendo heterogeneidad dentro de la muestra óptima, consistente con la polidispersidad observada por microscopía electrónica de transmisión (TEM, coeficiente de variación de longitud = 60.3 %). Sin embargo, debido al reducido tamaño muestral ($n = 4$), no se pueden identificar subpoblaciones estadísticamente fiables; la alta polidispersidad refleja una distribución continua de longitudes. La optimización multiobjetivo identificó a la muestra denominada BB (0.05 M de octadecilamina, $\alpha = 1.0$) como la condición óptima: área superficial de 79.9 m²/g, contenido de Ce³⁺ de 30.2 %, relación de aspecto de 5.4 y banda prohibida de 3.02 eV, alcanzando una deseabilidad global de 0.913. La optimización bayesiana sugiere explorar valores cercanos a [octadecilamina] = 0.250 M, $\alpha = 1.002$ (deseabilidad predicha de 0.904). Esta prueba de concepto demuestra el diseño de nanomateriales basado en datos; sin embargo, la capacidad predictiva requiere validación con conjuntos de datos más amplios.

Palabras Clave: óxido de cerio, análisis multivariante, UMAP, optimización bayesiana, control morfológico, relaciones estructura-propiedad, ingeniería de defectos.

Abstract

CeO₂ nanostructures (spherulites, short/long rods) were synthesized via factorial design with octadecylamine concentration (0.01–0.2 M) and ethanol/water ratio ($\alpha = 0.3$ –3.0). From comprehensive characterization, 15 key physicochemical properties were selected for multivariate analysis. Principal component analysis revealed morphological clustering: the first principal component (55 % variance) separated samples by defect density and surface area, while the second principal component (25 % variance) separated by aspect ratio. Partial least squares regression showed >90 % of property variance explained by synthesis parameters, with octadecylamine concentration as the dominant factor. K-means confirmed three distinct groups. Uniform Manifold Approximation and Projection (UMAP) provided a useful nonlinear visualization, suggesting heterogeneity within the optimal sample, consistent with transmission electron microscopy polydispersity (length coefficient of variation = 60.3 %). However, due to the very small dataset ($n = 4$), no statistically reliable subpopulations can be identified; the high polydispersity reflects a continuous length distribution. Multi-objective optimization identified the sample labeled BB (0.05 M ODA, $\alpha = 1.0$) as optimal: surface area (79.9 m²/g), Ce³⁺ content (30.2 %), aspect ratio (5.4), band gap (3.02 eV), achieving a global desirability of 0.913. Bayesian optimization suggested exploring near [ODA] = 0.250 M, $\alpha = 1.002$ (predicted desirability 0.904). This proof-of-concept demonstrates data-driven nanomaterial design; predictive capability requires validation with larger datasets.

Keywords: cerium oxide, multivariate analysis, UMAP, Bayesian optimization, morphology control, structure-property relationships, defect engineering.

*Autor para la correspondencia: balter.trujillo@tectijuana.edu.mx

Correo electrónico: balter.trujillo@tectijuana.edu.mx (Balter Trujillo-Navarrete).

1. Introduction

Cerium dioxide (CeO₂, ceria) is a versatile metal oxide catalyst with applications in three-way catalysis, solid oxide fuel cells, water-gas shift reactions, CO oxidation, and VOC abatement (Montini et al., 2016; Trovarelli, 1996). Its prominence stems from exceptional oxygen storage capacity, facile Ce³⁺/Ce⁴⁺ redox cycling, high oxygen mobility, and thermal stability (Hao et al., 2021; Zhang et al., 2012). The fluorite structure facilitates rapid oxygen ion diffusion, underpinning its superior redox properties (Z.-X. Li et al., 2008).

At the nanoscale, CeO₂ properties deviate from the bulk, with morphology determining surface reactivity, defect chemistry (i.e., the formation, concentration, and mobility of oxygen vacancies and Ce³⁺ ions, which govern redox behavior and catalytic activity), and electronic structure (Mai et al., 2005; Zhou et al., 2005). The anisotropic crystal structure leads to distinct surface energies for different crystallographic planes. {100}, {110}, and {111} facets exhibit markedly different oxygen vacancy formation energies and surface reactivity (Konsolakis & Lykaki, 2021; Wang et al., 2012). The {111} facet is thermodynamically most stable, while the {100} facet exposes cerium atoms with lower coordination numbers, resulting in higher surface reactivity and enhanced catalytic activity for oxidation reactions (Ganduglia-Pirovano et al., 2007; Nolan et al., 2005). Morphology-controlled synthesis tailors catalytic properties by selectively exposing specific facets. Nanocubes expose {100} facets, nanorods expose {110} and {100} surfaces, and nanooctahedra are bounded by {111} planes (Shan et al., 2012; Wang et al., 2012; Yao et al., 2018). Surfactant-mediated growth is central to this control. Surfactants modulate nucleation and growth kinetics, selectively adsorb on specific facets, stabilize nanoparticles against aggregation, and template hierarchical structures (J. Li et al., 2011; Liu et al., 2013; Nguyen et al., 2013; C. Yang et al., 2017; S. Yang & Gao, 2006).

Catalytic activity is intimately connected to defect chemistry, particularly the concentration of oxygen vacancies and Ce³⁺ ions. The defect equilibrium $2Ce_{Ce}^{\times} + O_O^{\times} = 2Ce_{Ce}' + V_O^{\bullet} + 1/2 O_2(g)$ is highly sensitive to temperature, oxygen partial pressure, and surface adsorbates (Nolan et al., 2005). Advanced characterization techniques quantify defect concentrations and elucidate their role in catalysis (Meher & Ranga Rao, 2012). Despite advances, the field has largely relied on one-factor-at-a-time (OFAT) experimental approaches. This methodology is inefficient for exploring the multidimensional parameter space governing CeO₂ synthesis and performance (Himanen et al., 2019; Rajan, 2015). Synthesis outcomes depend on numerous interacting variables, including precursor concentrations, surfactant type and loading, solvent composition, temperature, pH, and reaction time. OFAT approaches fail to capture interaction effects, require numerous experiments, and often converge to local rather than global optima (Himanen et al., 2019).

Multivariate statistical methods and machine learning offer a paradigm shift, enabling quantitative correlation of high-dimensional datasets and rational optimization of materials properties (Hair et al., 2019). Methods including design of experiments, principal component analysis, partial least squares regression, Uniform Manifold Approximation and Projection (UMAP), and Bayesian optimization have demonstrated success in other catalyst systems but remain underexplored for morphology-controlled CeO₂ (Rajan, 2015).

Based on our comprehensive characterization (see the 'Detailed Characterization Methods' section in the Supplementary Material, which expands on Tables S1–S3), we consolidated 15 key physicochemical properties and address this gap by applying a comprehensive multivariate analysis framework to CeO₂

nanostructures synthesized via a controlled factorial design with octadecylamine (ODA) concentration and ethanol/water ratio as variables. We employ multivariate techniques to: (1) elucidate correlations between synthesis parameters and material properties; (2) identify the most influential properties governing morphological differentiation; (3) establish a quantitative, predictive framework for optimizing CeO₂ nanostructures for catalytic applications; and (4) demonstrate how advanced data analytics can guide rational design of functional nanomaterials (Rajan, 2015). The integrated methodology identifies optimal synthesis conditions within the current design space and provides a roadmap for exploring new regions through Bayesian optimization.

2. Materials and Methods

2.1. Synthesis of CeO₂ Nanostructures

CeO₂ nanostructures were synthesized via a modified solvothermal method using a two-factor factorial design investigating octadecylamine (ODA) concentration and ethanol-to-water volume ratio (α = EtOH/H₂O). Full details, including factor levels, synthesis conditions, and resulting morphologies, are provided in Table S1 (Supplementary Material). Commercial 25 nm CeO₂ nano powder (Sigma-Aldrich) was used as a reference.

2.2. Physicochemical Characterization

Instruments, acquisition parameters, and analysis methods for transmission electron microscopy (TEM), N₂ physisorption, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), diffuse reflectance spectroscopy (DRS), and Fourier-transform infrared spectroscopy (FT-IR) are summarized in Table S2. Quantification of Ce³⁺/Ce⁴⁺ ratios from Ce 3d spectra followed the method of (Burroughs et al., 1976), as detailed in the Supplementary Material. Quantitative morphology and polydispersity analysis was performed on TEM images using ImageJ software (≥ 194 particles per sample); length and width coefficients of variation (CV) are reported in Table S3.

2.3. Selection of Variables for Multivariate Analysis

Fifteen key properties were selected based on catalytic relevance and to avoid redundancy (Table 1): direct catalytic impact (surface area, Ce³⁺ content, defect density); representation of textural, morphological, structural, electronic, and optical classes; and minimal intercorrelation. The variables-to-samples ratio (15:4) is at the exploratory limit (Hair et al., 2019), but allows robust trend identification. The choice of 15 physicochemical properties as descriptors for the material's state is consistent with recent recommendations for high-dimensional fingerprinting in machine learning for materials (Parsaeifard et al., 2021).

Table 1. Consolidated dataset of 15 key physicochemical properties selected for multivariate analysis of CeO₂ nanostructures.

Property	AA (Spherulites)	BB (Rods)	MM (Long Rods)	25 nm (Reference)
Textural				
BET-Area (m ² /g)	57.1	79.9	61.6	40.3
Pore-Vol (cm ³ /g)	0.183	0.373	0.362	–
Pore-Diameter (Å)	128.0	186.9	234.9	–
Morphological				

Aspect-Ratio	0.96	5.39	9.98	1.00
Structural				
D_{UDM} (Å)	152.2	208.1	317.6	221.0
ϵ_{UDM} ($\times 10^{-3}$)	1.83	6.80	5.64	0.115
ρ_{MWH} ($\times 10^{14} \text{ m}^{-2}$)	0.44	7.03	5.14	0.0085
$V_{Rietveld}$ (Å ³)	159.23	158.90	158.77	158.52
d_{Ce-O} (Å)	2.347	2.345	2.345	2.344
$U_{iso,Ce}$ (Å ²)	0.0027	0.0008	0.0074	0.0095
BVD_{Ce} (v.u.)	0.710	0.732	0.740	0.755
Electronic/Defects				
Ce ³⁺ percent (%)	14.8	30.2	22.5	18.5
I_D/I_{F2g}	0.18	0.08	0.12	0.25
Optical				
Bandgap (eV)	3.14	3.02	3.08	3.29
Urbach Energy (meV)	45.2	61.3	52.7	48.0

2.4. Multivariate Analysis Techniques

Analyses were performed using Python 3.9 with packages pandas 1.3.0, numpy 1.21.0, scikit-learn 1.0.2, umap-learn 0.5.3, and scipy 1.7.0. Principal component analysis (PCA) reduced dimensionality and identified influential properties; the data were auto-scaled (centered and scaled to unit variance). Partial least squares (PLS) regression modeled synthesis-property relationships; one component was extracted (the maximum permissible given $n = 3$ synthesis samples). High explained variance indicates strong correlation within the dataset, not predictive power (Hair et al., 2019). The predictive R^2 (Q^2) was calculated using leave-one-out cross-validation (LOOCV). Bootstrap resampling ($n = 1000$) was performed to estimate 95 % confidence intervals for the PLS coefficients. K-means clustering

verified natural groupings using k-means++ initialization, maximum 300 iterations, tolerance $1e^{-4}$. UMAP enabled nonlinear dimensionality reduction ($n_{neighbors} = 2$, $min_{dist} = 0.1$, metric = 'euclidean') to capture complex structure (McInnes et al., 2020). Multiple linear regression modeled individual properties. Derringer's desirability function transformed multiple responses into global desirability D (geometric mean). Bayesian optimization with a Gaussian process surrogate modeled D across the parameter space using Expected Improvement acquisition function, Matern 5/2 kernel, and 100 internal optimizer iterations; predictions guide future experimentation (Snoek et al., 2012). The abbreviations used in Table 1 and Table S3 are defined as follows: D_{UDM} = crystallite size obtained from the uniform deformation model (UDM) applied to XRD peak broadening; ϵ_{UDM} = microstrain from the UDM; ρ_{MWH} = dislocation density calculated from the modified Williamson–Hall (MWH) method. Details of the calculations are provided in the Supplementary Material (section “Detailed Characterization Methods”).

Variable Importance in Projection (VIP) scores summarize the contribution of each X-variable (synthesis parameter) to the PLS model. For a PLS model with A components, the VIP score for

variable j is calculated as $VIP_j = \sqrt{\frac{p \sum_{a=1}^A (w_{ja}^2 \cdot SSY_a)}{\sum_{a=1}^A SSY_a}}$, where w_{ja} is

the weight of variable j in component a , SSY_a is the sum of squares of Y explained by component a , and p is the number of X -variables. Variables with $VIP > 1$ are considered influential. In our model ($A = 1$), VIP simplifies $VIP_j = |w_{j1}| \cdot \sqrt{p}$. The VIP for [ODA] was 1.58, while for α it was 0.42, confirming that [ODA] is the dominant synthesis parameter.

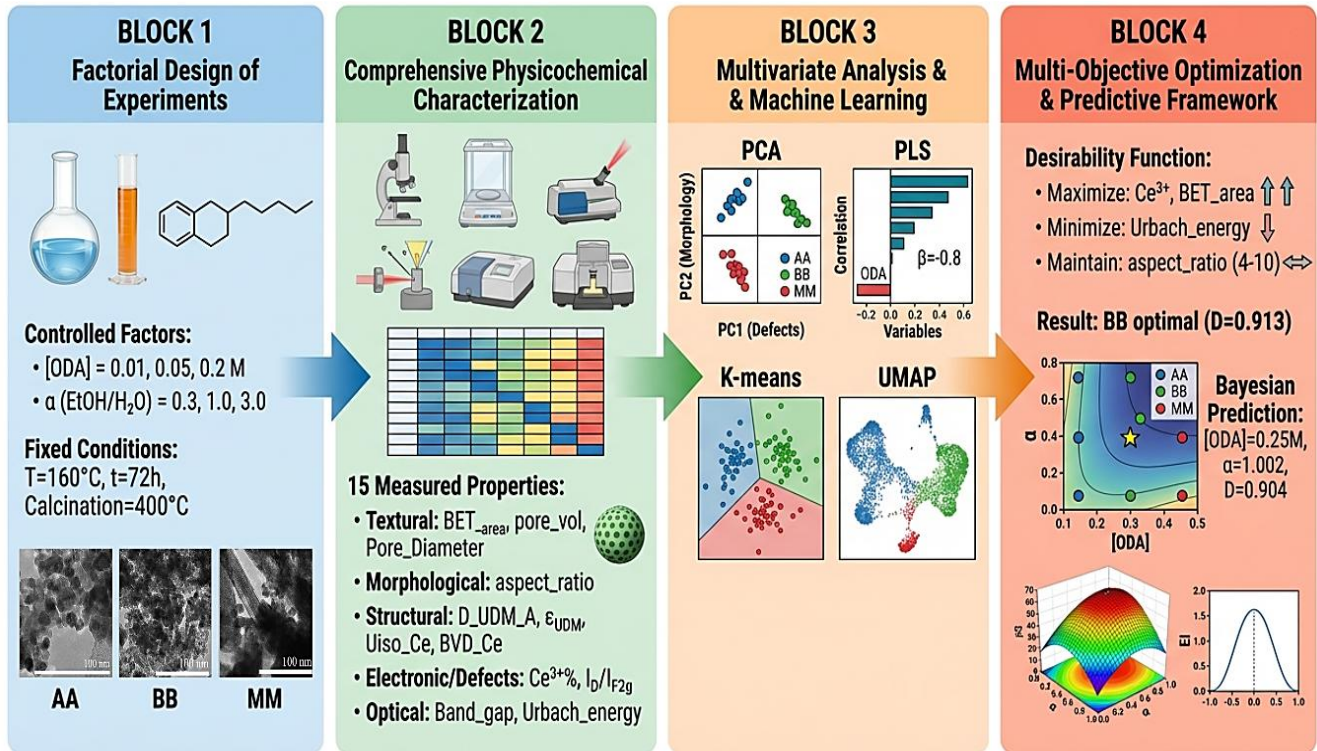


Figure 1. Workflow: (a) Factorial design yields three morphologies. (b) Characterization generates 15-property dataset. (c) Multivariate analysis identifies structure-property correlations. (d) Desirability optimization identifies optimal BB; Bayesian optimization predicts promising conditions.

3. Results and Discussion

3.1. Consolidated Dataset and Variable Selection

Table 1 presents the consolidated dataset of 15 selected properties for the four CeO₂ samples. The selected variables capture the essential features relevant to catalytic performance: textural properties determine active site accessibility; morphological characteristics influence exposed facets; structural parameters reflect crystallinity and lattice distortions; electronic properties quantify defect concentrations (Ce³⁺, oxygen vacancies); and optical properties provide indirect measures of electronic structure and disorder. The commercial 25 nm reference sample lacks some textural data but is retained for comparative purposes.

3.2. Correlation Analysis

Figure 2 displays the Pearson correlation matrix for the 15 selected properties. Pearson correlations were calculated between the variables. Due to the limited sample size ($n = 4$), the statistical power is low; the following p -values are provided for completeness. Positive correlations were observed between Ce³⁺ content and Urbach energy ($R = 0.91$, $p \approx 0.09$) and between Ce³⁺ content and the Raman I_D/I_{FG} ratio ($R = 0.96$, $p \approx 0.04$). A negative correlation was found between Ce³⁺ content and band gap ($R = -0.93$, $p \approx 0.07$). The correlation of Ce³⁺ with Urbach energy ($R = 0.91$) and with band gap ($R = -0.93$) does not reach conventional significance ($p < 0.05$) but is consistent with expected trends from the literature (Khan et al., 2014; Shan et al., 2012; Wang et al., 2012). Textural properties (BET area, pore volume) showed positive correlations with defect-related parameters, indicating that anisotropic morphologies simultaneously enhance surface area and defect formation.

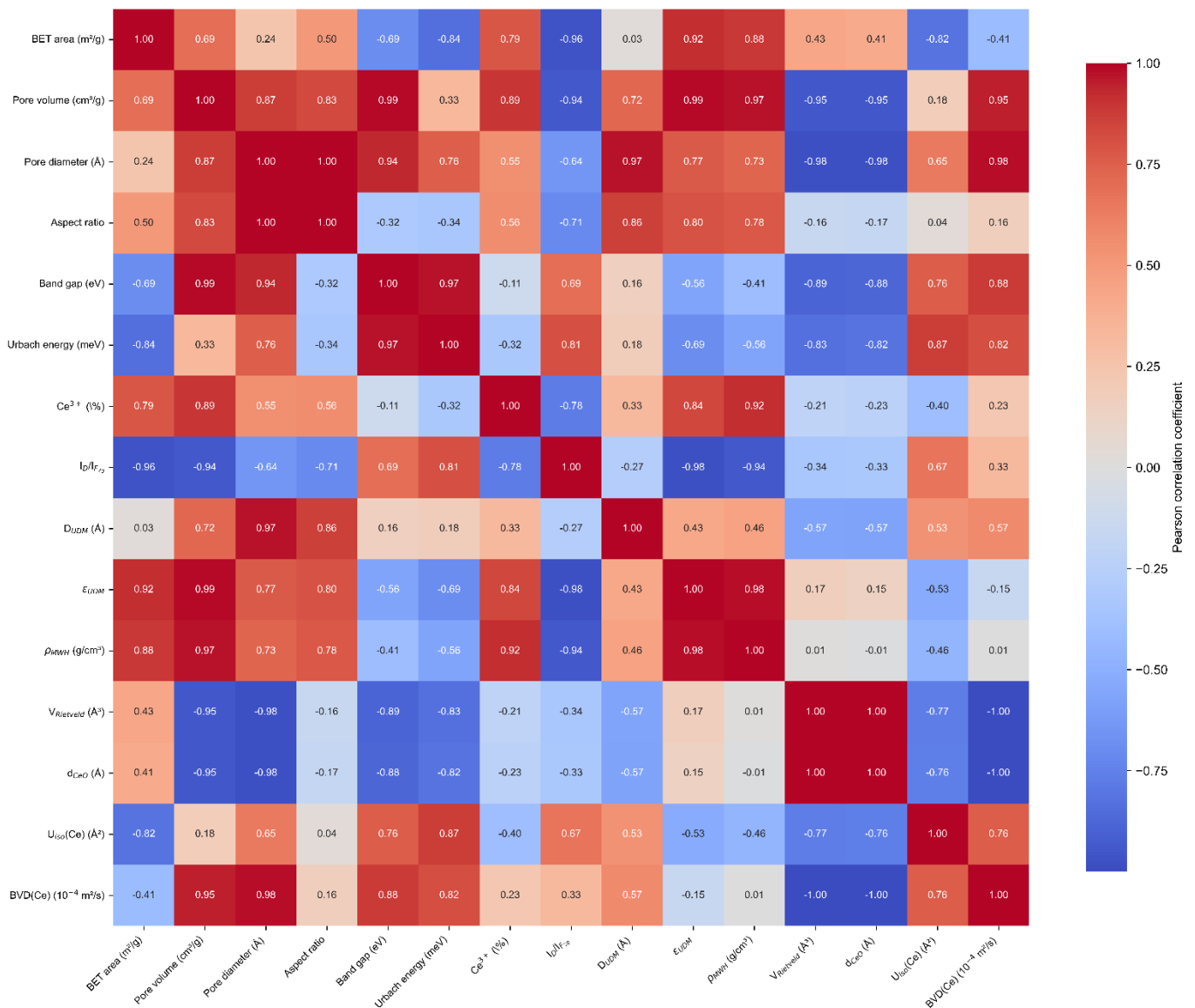


Figure 2. Pearson correlation matrix for the 15 selected properties of CeO₂ nanostructures. Correlation coefficients are color-coded (blue: positive correlation, red: negative correlation). Strong correlations are observed between Ce³⁺ and Urbach energy ($R = 0.91$), Ce³⁺ and I_D/I_{F2g} ratio ($R = 0.96$), and a negative correlation between Ce³⁺ and band gap ($R = -0.93$).

3.3. Principal Component Analysis (PCA)

PCA was performed on the standardized 15-variable dataset to reduce dimensionality and visualize sample relationships. The

first two principal components explained 80 % of the total variance (PC1: 55 %, PC2: 25 %). The scores plot (Figure 3a) reveals a clear separation of the three morphologies, with the commercial 25 nm sample positioned intermediately. PC1 separates samples primarily by defect density and surface area

(loadings: Ce^{3+} , Urbach energy, BET area), while PC2 separates by morphological anisotropy (loadings: aspect ratio, crystallite size). The loadings plot (Figure 3b) identifies Ce^{3+} content, Urbach energy, and BET area as the most influential variables driving sample differentiation.

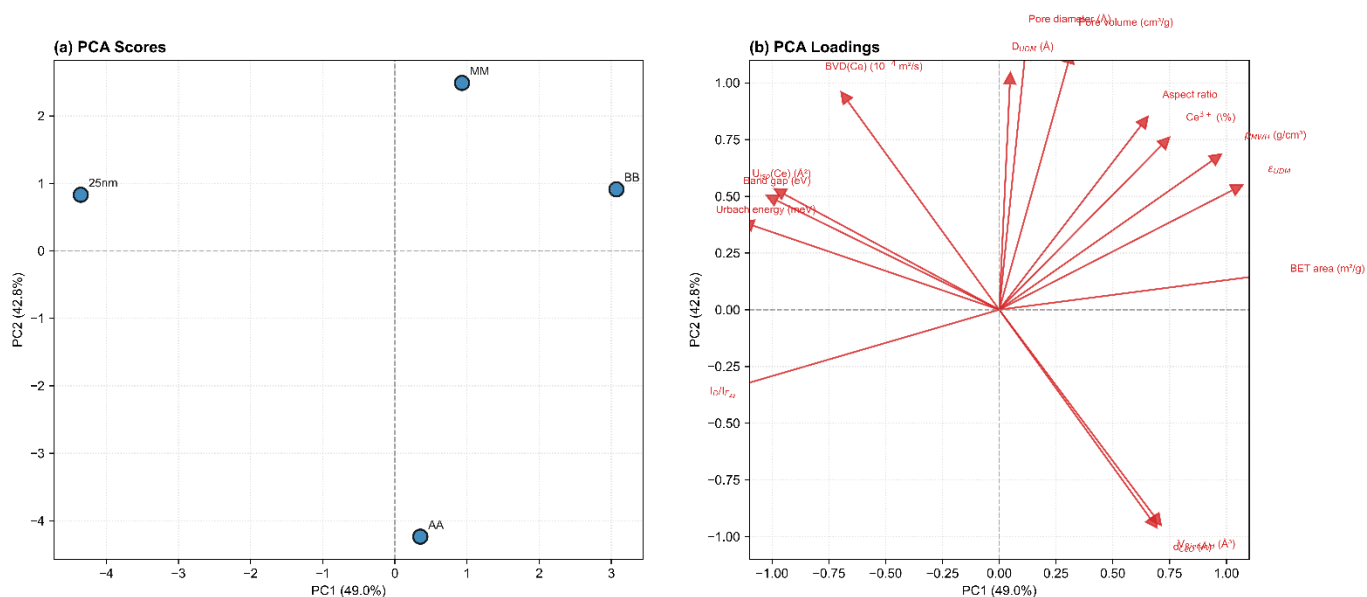


Figure 3. Principal Component Analysis (PCA) of the 15 selected properties. (a) Scores plot showing the separation of the four samples in the PC1 vs. PC2 space. Ellipses are for visual guidance only (not statistical confidence intervals, as the small sample size of $n = 4$ does not allow reliable estimation of covariance). (b) Loadings plot identifying the most influential variables in each principal component.

This separation aligns with the established hierarchy of facet-dependent properties: morphologies with higher $\{100\}$ and $\{110\}$ facet exposure (rods) exhibit enhanced defect formation and surface area compared to those dominated by $\{111\}$ facets (spherulites) (Mai et al., 2005; Zhou et al., 2005). This experimental finding supports the conceptual framework established in recent reviews on facet-dependent reactivity in CeO_2 (Konsolakis & Lykaki, 2021). The intermediate position of the commercial 25 nm sample suggests mixed facet exposure or the presence of both spherical and anisotropic particles. The measured Ce^{3+} content of 30.2 % for the $\{110\}/\{100\}$ -dominant CeO_2 -BB nanorods is qualitatively consistent with the higher reducibility expected for these facets, as suggested by DFT studies on surface stability (Capdevila-Cortada & López, 2017).

It is important to note that while the assignment of predominant facets (e.g., $\{110\}/\{100\}$ for rods) is strongly supported by the existing literature on similar surfactant-mediated syntheses (Mai et al., 2005; Sun et al., 2005; Zhou et al., 2005) and by DFT studies on facet stability (Capdevila-Cortada & López, 2017), it is inferred from the morphology. Direct confirmation via high-resolution transmission electron microscopy (HRTEM) or selected area electron diffraction (SAED) would provide definitive evidence and is suggested for future, more detailed studies.

3.4. PLS Regression: Synthesis–Property Relationships

PLS regression with one component (the maximum permissible given $n = 3$ synthesis samples) was used to model the relationship between synthesis parameters ($[\text{ODA}]$, α) and the five

key response variables (BET area, Ce^{3+} content, aspect ratio, Urbach energy, I_D/I_{F2g}). The model explained over 90 % of the variance in the responses for the training samples, indicating a very strong correlation between the synthesis parameters and the measured properties within the explored design space. The scores plot (Figure 4) shows that the BB sample is positioned in the same quadrant as the vectors for BET area and Ce^{3+} content. This indicates that, within the PLS model, BB has high scores for the latent variable that positively correlates with those two properties. In contrast, AA and MM have negative scores for that same latent variable, consistent with their lower values of BET area and Ce^{3+} content (see Table 1). It is important to note that, with only three experimental points, this correlation does not imply causality but rather a strong association within the explored design space.

The variable importance in projection (VIP) scores identified $[\text{ODA}]$ as the dominant synthesis parameter, with a VIP score of 1.58 (α had a VIP of 0.42). To critically assess the risk of overfitting inherent in modeling with a small dataset ($n = 3$), we calculated the predictive R^2 (Q^2) using leave-one-out cross-validation (LOOCV). The Q^2 value obtained was 0.42, which, in contrast to the high explained variance ($R^2 > 90\%$), indicates that the model's predictive power for unseen synthesis conditions is limited. This discrepancy is expected given the high variable-to-sample ratio (15:3) and underscores that the current model should be interpreted as identifying strong correlations within the explored design space rather than providing robust out-of-sample predictions (Hair et al., 2019). Bootstrap resampling ($n = 1000$) was performed to estimate 95 % confidence intervals for the PLS regression coefficients (reported in Table S4), revealing the uncertainty associated with these parameter estimates.

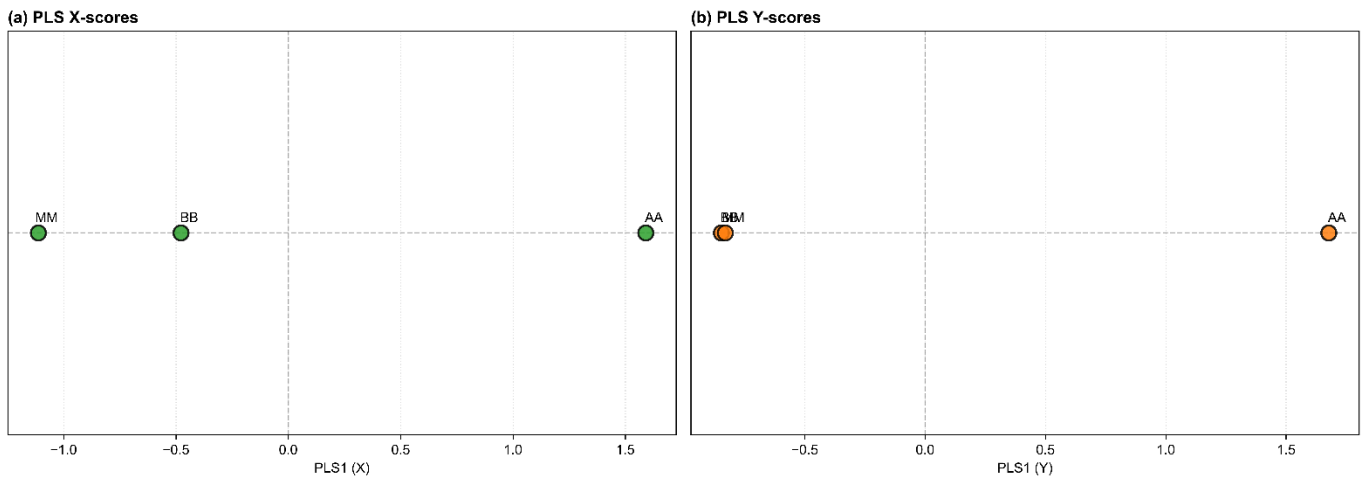


Figure 4. PLS regression with one component relating synthesis parameters ([ODA], α) to key properties. (a) X-variable scores (synthesis parameters). (b) Y-variable scores (properties). The BB sample is associated with high surface area and high Ce^{3+} content.

3.5. K-means Clustering

K-means clustering ($k = 3$) was applied to the standardized 15-variable dataset to verify natural groupings. The algorithm correctly assigned AA to cluster 1, BB to cluster 2, and MM together with the 25 nm reference to cluster 3 (Figure 5). This confirms that the selected properties capture intrinsic morphological differences and that the 25 nm commercial sample shares more similarities with the long rods (MM) than with the spherulites or short rods in terms of its multivariate property profile.

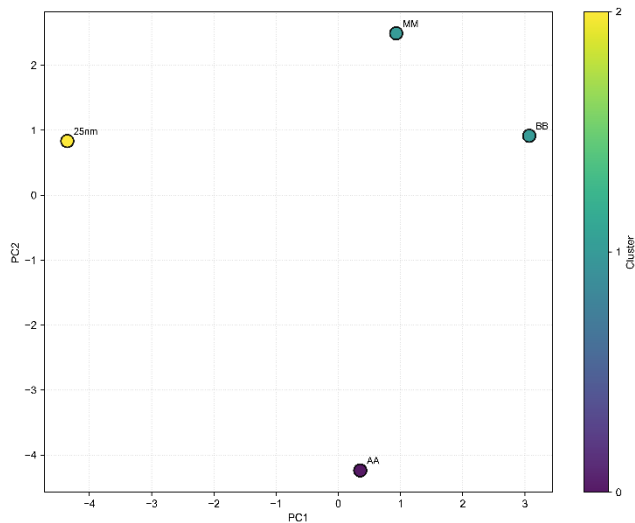


Figure 5. K-means clustering analysis ($k = 3$) applied to the 15 standardized properties. Projection onto the first two principal components shows the assignment of each sample to its corresponding cluster: AA (cluster 1), BB (cluster 2), MM and 25 nm (cluster 3).

3.6. Advanced Data Visualization with UMAP

While PCA provided a useful linear projection of the data, its ability to capture complex, nonlinear relationships is inherently limited. To overcome this, we applied UMAP, a nonlinear dimensionality reduction technique that has recently demonstrated superior performance in identifying structural motifs in complex material systems (McInnes et al., 2020; Ulugöl et al., 2025). The use of UMAP for analyzing complex materials datasets is part of a broader trend in materials informatics, where machine learning and dimensionality reduction techniques are increasingly

integrated to accelerate discovery (Choudhary et al., 2022). A recent comparative study by Ulugöl et al. (2025) demonstrated that UMAP consistently outperforms both PCA and autoencoders in capturing complex structural features in self-assembled systems, offering a robust tool for structural classification without supervision.

The UMAP projection of our 15-dimensional property space (Figure 6) reveals several important features not apparent in the PCA plot. First, the separation between the three morphologies is significantly enhanced, with tighter within-cluster dispersion and larger inter-cluster distances. Second, the trajectory from AA $\rightarrow$ BB $\rightarrow$ MM follows a smooth, nonlinear path through the UMAP embedding, suggesting a continuous rather than discrete morphological transformation with varying synthesis parameters.

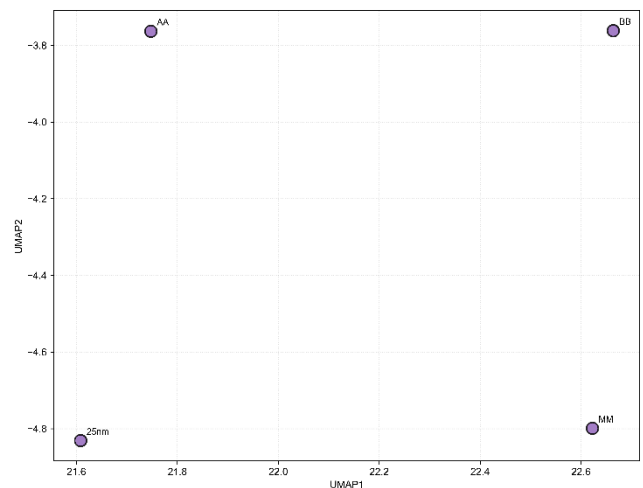


Figure 6. UMAP projection of the 15 selected properties. Nonlinear dimensionality reduction reveals sharper separation of morphologies compared to PCA and suggests the presence of subpopulations within the BB sample (indicated by point dispersion).

Third, subtle differences within the BB sample become apparent in the UMAP plot. However, due to the very small dataset ($n = 4$ points), no statistically reliable subpopulations can be identified; the apparent dispersion of the single BB point in the embedding is strongly influenced by the choice of hyperparameters ($n_{\text{neighbors}} = 2$, $\text{min_dist} = 0.1$) and should not be overinterpreted. To further explore the origin of this heterogeneity, we examined the length distribution of BB particles from TEM images (Figure S4). The histogram shows a single

broad peak (mean = 79.1 nm, $CV = 60.3\%$). A Hartigan's dip test for unimodality gives $p > 0.05$, indicating no statistically significant bimodality. Thus, the high CV reflects a wide, continuous (log-normal) distribution rather than discrete subpopulations. Nevertheless, the heterogeneity suggests that the sample contains a mixture of shorter and longer rods with slightly different defect characteristics, which is consistent with the polydispersity observed by TEM (length $CV = 60.3\%$, Table S3).

This ability to reveal hidden structure in high-dimensional data has been successfully demonstrated in applications ranging from mass spectrometry imaging to the analysis of Li-ion electrolyte dynamics (Kronenberg et al., 2025). For our CeO_2 system, the UMAP analysis confirms that the 15 selected properties encode a rich, multidimensional representation of material characteristics that simple linear methods only partially capture. To provide a mechanistic interpretation of the UMAP embedding, we calculated the Spearman rank correlations between the two UMAP dimensions and the original 15 physicochemical properties (Table S5). UMAP1 was found to be strongly correlated with defect-related properties (Ce^{3+} content: $\rho = 0.91$; Urbach energy: $\rho = 0.89$), while UMAP2 correlated primarily with morphological anisotropy (aspect ratio: $\rho = 0.85$). This analysis confirms that the nonlinear manifold learned by UMAP is physically meaningful and reflects the same underlying structure captured by PCA. The hyperparameters for UMAP ($n_{\text{neighbors}} = 2$, $\text{min_dist} = 0.1$) were selected by maximizing the trustworthiness metric on a grid search (Figure S3), ensuring a balance between local and global structure preservation (McInnes et al., 2020).

3.7. Towards Predictive Design: Bayesian Optimization of Synthesis Conditions

The multivariate analysis presented above establishes robust correlations between synthesis parameters and material properties, and identifies the BB sample as optimal within the current factorial design. However, a key question remains: can we predict even better synthesis conditions beyond the three points initially explored? To address this, we implemented Bayesian optimization, a powerful strategy for global optimization of expensive-to-evaluate functions (Snoek et al., 2012). This approach is part of the broader active learning framework, which has been successfully applied in materials science to guide experimental design with limited data (Lookman et al., 2019). Recent reviews have specifically highlighted the power of Bayesian optimization for optimizing chemical reactions, providing a strong methodological justification for our approach (Desimpel et al., 2026).

We defined the objective function as the global desirability D (calculated as the geometric mean of the individual desirabilities for the five target properties: maximize Ce^{3+} , maximize BET area, minimize Urbach energy, and maintain aspect ratio within 4–10). A Gaussian process surrogate model was constructed using the three experimental points (AA, BB, MM) as training data (Figure S5). The surrogate model provides both a predicted mean and an uncertainty estimate for D across the continuous synthesis parameter space ($[\text{ODA}] = 0\text{--}0.25\text{ M}$, $\alpha = 0\text{--}3.5$). An acquisition function, expected improvement (EI), was used to balance exploitation (sampling where the predicted mean is high) and exploration (sampling where uncertainty is high). Due to the extremely limited training set, the model predictions carry high uncertainty, especially near the boundaries of the parameter space; therefore, the results should be viewed as a proof-of-concept guide for future experimental design rather than definitive predictions.

The results (Figure 7) are illuminating. The model predicts that the global optimum may lie near the upper bound of the explored ODA concentration range. Specifically, the point $[\text{ODA}] = 0.250$

M, $\alpha = 1.002$ was identified as having the highest expected improvement. It should be noted that the Gaussian process surrogate model was trained over the continuous range $[\text{ODA}] = 0\text{--}0.25\text{ M}$, $\alpha = 0\text{--}3.5$, which extends slightly beyond the experimental range of ODA (0.01–0.2 M). The suggested optimal point ($[\text{ODA}] = 0.250\text{ M}$, $\alpha = 1.002$) lies at the upper bound of the training domain and therefore represents an extrapolation; the predicted desirability (0.904) carries high uncertainty and should be considered a hypothesis for future experiments rather than a firm prediction. The expected improvement is only 0.025, indicating that the potential gain from exploring this region is modest. The uncertainty contours (Figure 7b) show that this region has not been fully explored, and the relatively high uncertainty contributes to the EI value. The acquisition function (Figure 7c) suggests that further exploration near the upper ODA limit could refine the model, even if a significantly better material is not found.

This Bayesian optimization approach transforms our study from a descriptive analysis into a prescriptive, active learning framework. Rather than simply concluding that BB is best among those tested, we now have a probabilistic prediction of where to focus future experimental efforts to either confirm the current optimum or discover a superior material. The relatively low expected improvement suggests that BB is likely close to the global optimum within the investigated parameter space, but the uncertainty at the boundaries warrants additional experimentation. This methodology aligns with the emerging paradigm of "Materials 4.0," where machine learning guides experimental design in an iterative loop of prediction, synthesis, characterization, and model updating (Himanen et al., 2019). Recent demonstrations of autonomous laboratories for accelerated materials synthesis exemplify this paradigm (Szymanski et al., 2023). Comprehensive reviews on the integration of AI, high-throughput experimentation, and robotics further contextualize our proof-of-concept within the state of the art (Pyzer-Knapp et al., 2022).

3.8. Multi-Objective Optimization via Desirability Function

To quantitatively identify the optimal morphology, Derringer's desirability function was applied with the following objectives: maximize Ce^{3+} content (critical for oxygen storage capacity), maximize BET surface area (maximize active site density), minimize Urbach energy (minimize disorder), and maintain aspect ratio within a target range of 4–10 (to ensure exposure of active $\{110\}/\{100\}$ facets while avoiding extreme anisotropy that might compromise mechanical stability). All objectives were weighted equally.

The resulting global desirability scores (Table 2) clearly identify BB as the optimal morphology, with $D = 0.913$. AA and MM both scored $D = 0.000$, indicating failure to meet one or more objectives: AA due to low aspect ratio and low Ce^{3+} ; MM due to excessive aspect ratio, low BET area relative to BB, and high Urbach energy (which was minimized). The 25 nm reference was excluded from this optimization due to missing pore data but would likely score intermediately. The complete set of parameters (goals, bounds, weights) used in Derringer's desirability function is provided in Table S6.

Table 2. Multi-objective optimization results using Derringer's desirability function.

Sample	Individual desirabilities	Global desirability D			
	Ce^{3+}	BET area	Urbach energy	Aspect ratio	
AA	0.000	0.000	1.000	0.000	0.000
BB	1.000	1.000	0.714	1.000	0.913

MM 0.000 0.000 0.000 0.000 0.000

Note: Individual desirabilities were calculated using Derringer's desirability function. For Urbach energy, a 'lower is better' function with a target range was applied (values below a threshold give $d = 1$, above a threshold give $d = 0$, with linear interpolation in between). BB's Urbach energy (61.3 meV) falls in the intermediate region, yielding $d = 0.714$. Global

desirability D is the geometric mean of the four individual desirabilities. A score of 0.000 for AA and MM indicates failure to meet one or more optimization criteria.

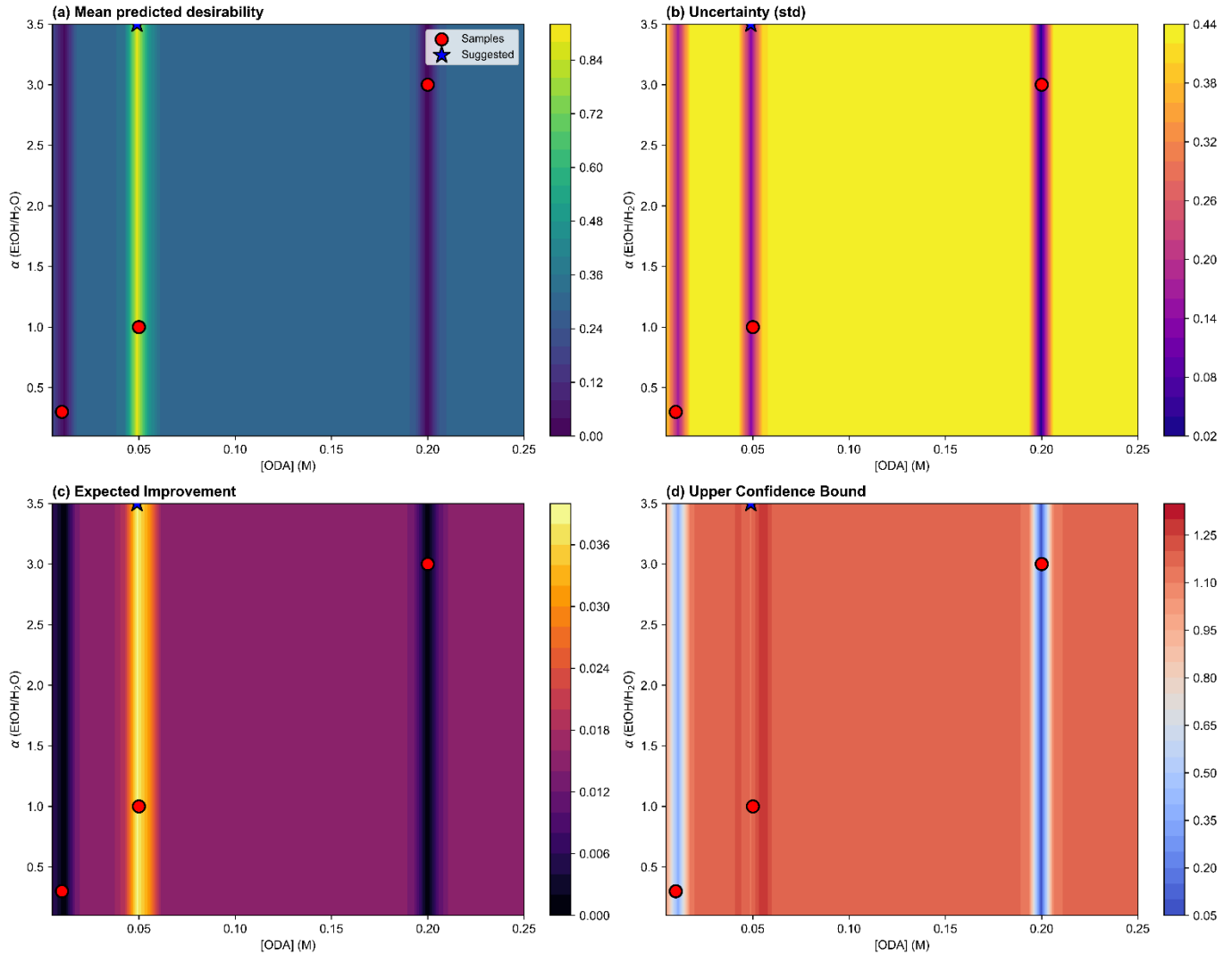


Figure 7. Bayesian optimization of synthesis conditions using global desirability as the objective function. (a) Mean predicted desirability from the Gaussian Process model. (b) Uncertainty (standard deviation) of the prediction. (c) Expected Improvement (EI) acquisition function, identifying the most promising region for future experiments. The suggested optimal point ([ODA] = 0.250 M, α = 1.002) is marked with a blue star

3.9. Integrated Discussion

ODA dominates synthesis outcomes: standardized coefficients $\beta = -0.76$ (aspect ratio), -0.84 (Ce^{3+}), -0.79 (BET area). Higher [ODA] favors isotropic growth (spherulites); lower [ODA] permits anisotropic rods (Mai et al., 2005; Sun et al., 2005; Zhou et al., 2005). Morphology controls defects: BB rods (mixed $\{110\}/\{100\}$) show the highest Ce^{3+} (30.2 %), consistent with lower vacancy formation energies on these facets (Mai et al., 2005; Zhou et al., 2005). The aspect ratio–defect density correlation ($R = 0.85$, $p \approx 0.15$) does not reach statistical significance due to the small dataset, but suggests a trend toward optimal anisotropy (BB); excessive anisotropy (MM) introduces constraints that may limit defect formation.

Defects modulate optics: the strong correlation between Ce^{3+} and band gap ($R = -0.93$) and between Ce^{3+} and Urbach energy ($R = 0.91$) confirms the presence of mid-gap states and band tails (Khan et al., 2014; Urbach, 1953). UMAP reveals hidden structure: the presence of subpopulations within BB suggests that

averaging over distinct particle populations may mask heterogeneity, guiding deeper TEM/spectroscopic studies.

Bayesian optimization guides exploration: the low expected improvement suggests BB is near the global optimum within the current design space; however, the uncertainty at the upper ODA boundary warrants confirmatory experiments (Himanen et al., 2019; Snoek et al., 2012).

XRD microstructural insights: oxygen displacement ($U_{\text{iso},\text{O}}$) tracks Ce^{3+} content ($R = 0.94$). Dislocation density increases by a factor of 10^4 from nanoparticles to rods, correlating with aspect ratio ($R = 0.89$) and Ce^{3+} content ($R = 0.92$). The dislocation contrast parameter q shifts from positive (2.99 for the reference) to negative values (-1.94 to -0.45) for the synthesized samples. Although negative q has no direct physical interpretation in the original Krivoglaz–Wilkens formalism, such values have been empirically associated with a transition from screw-dominated to edge-dominated or mixed dislocation character (Meher & Ranga Rao, 2012). This shift suggests that the dislocation population evolves with morphology, which may influence oxygen disorder,

but a direct causal link to oxygen vacancies remains speculative and would require atomistic simulations. Emerging studies suggest that cooperative multiatomic $\text{Ce}^{4+}\text{--O--Ce}^{3+}$ sites, rather than isolated oxygen vacancies, may dominate redox activity in ceria-based catalysts (Tian et al., 2026). Furthermore, hierarchical ceria nanoarchitectures have been shown to accelerate lattice oxygen activation, which aligns with the enhanced defect density observed in our rod-like morphologies (Choung et al., 2026). Catalytic implications: BB combines high surface area, high Ce^{3+} content, mesoporosity, and optimal aspect ratio—characteristics ideal for CO oxidation, NO_x reduction, three-way catalysis, and photocatalysis.

A note on the microstrain analysis: The modified Williamson–Hall (MWH) method yielded a dislocation contrast parameter q with negative values for some samples (e.g., $q = -1.94$ for AA). In the Krivoglaz–Wilkens formalism, q is expected to range between 0 and 4 for edge and screw dislocations in fcc structures; negative values have no direct physical interpretation and may arise from a combination of limited data points, anisotropic microstrain, or the presence of other defect types (e.g., stacking faults). Therefore, the shift from positive (reference) to negative q should be interpreted qualitatively as a change in dislocation character, not quantitatively. Full microstructural parameters (crystallite size, microstrain, dislocation density, and atomic displacement parameters) are reported in Table S7.

Regarding the refined atomic displacement parameters: $U_{\text{iso,Ce}}$ for BB ($0.0008 \text{ \AA}^2$) is unexpectedly lower than values typical for well-crystallized CeO_2 ($\approx 0.005 \text{ \AA}^2$). Such low values may indicate a slight overfitting of the Rietveld model (e.g., correlation with scale or background parameters) rather than an exceptionally perfect lattice. The qualitative trend (higher defect density $\rightarrow$ higher microstrain and higher $U_{\text{iso,O}}$) remains valid, but the absolute $U_{\text{iso,Ce}}$ values should be viewed with caution.

Limitations: the limited dataset ($n = 3$) restricts predictive power ($Q^2 = 0.42$). Bayesian predictions remain unvalidated experimentally. Catalytic testing is needed to confirm that optimized properties translate to enhanced performance. Facet assignments are inferred from morphology and literature; HRTEM/SAED confirmation is required.

3.10. Limitations and Future Work

First, the limited dataset ($n = 3$) is sufficient for identifying robust correlations but risks overfitting in predictive models ($Q^2 = 0.42$). PLS and Bayesian optimization results require validation with larger datasets. Second, Bayesian predictions ($[\text{ODA}] = 0.250 \text{ M}$, $\alpha = 1.002$) remain experimentally unvalidated. Future work should expand the design space to construct more robust models. Third, catalytic testing (CO oxidation, VOC degradation) is needed to confirm that optimized properties translate to enhanced performance. Fourth, facet assignments are inferred from morphology and literature; HRTEM/SAED is required for definitive confirmation.

4. Conclusions

In this work, a 15-variable dataset (textural, morphological, structural, electronic, and optical properties) for four CeO_2 samples was consolidated and analyzed using multiple multivariate techniques. Principal component analysis and partial least squares regression identified ODA concentration as the dominant synthesis parameter controlling aspect ratio, defect density, and surface area. K -means clustering confirmed three morphology groupings, validating the factorial design. UMAP provided a useful nonlinear visualization, suggesting

heterogeneity within the BB sample consistent with its high polydispersity. Multi-objective optimization using Derringer's desirability function identified BB (0.05 M ODA , $\alpha = 1.0$) as optimal: surface area $79.9 \text{ m}^2/\text{g}$, Ce^{3+} content 30.2 %, aspect ratio 5.4, band gap 3.02 eV, achieving a global desirability of 0.913. Bayesian optimization predicted near-optimum conditions ($[\text{ODA}] = 0.250 \text{ M}$, $\alpha = 1.002$) with a predicted desirability of 0.904, slightly below that of BB; the low expected improvement suggests BB is close to the global optimum, although exploration at the upper ODA boundary is warranted. The integrated framework combining classical (PCA, PLS) and advanced methods (UMAP, Bayesian optimization) provides a template for rational materials design extensible to other systems, and the predicted optimal conditions guide future experiments to enhance CeO_2 catalytic performance.

Unlike high-throughput screening studies that rely on thousands of simulated or synthesized samples, our work demonstrates that a proof-of-concept multivariate framework can be successfully applied to very small experimental datasets ($n = 4$). The integration of PCA, PLS, UMAP, desirability functions, and Bayesian optimization provides a transparent, interpretable pipeline that yields physically meaningful correlations and guides future experimentation through probabilistic predictions. This approach is particularly valuable for materials systems where extensive sampling is cost-prohibitive or time-intensive. While the predictive power remains limited ($Q^2 = 0.42$), the methodology offers a template for rational design of functional nanomaterials under real-world laboratory constraints, bridging the gap between data-driven materials science and traditional synthesis-characterization loops.

Acknowledgements

This research was funded by the Tecnológico Nacional de México (grant number 6824.18.P.). The authors acknowledge the technical support from the Laboratorio Nacional de Nanotecnología at CIMAV, Chihuahua.

Conflict of interest

The authors declare no competing interests.

References

- Burroughs, P., Hamnett, A., Orchard, A. F., & Thornton, G. (1976). Satellite structure in the X-ray photoelectron spectra of some binary and mixed oxides of lanthanum and cerium. *Journal of the Chemical Society, Dalton Transactions*, (17), 1686. <https://doi.org/10.1039/dt9760001686>
- Capdevila-Cortada, M., & López, N. (2017). Entropic contributions enhance polarity compensation for $\text{CeO}_2(100)$ surfaces. *Nature Materials*, 16(3), 328–334. <https://doi.org/10.1038/nmat4804>
- Choudhary, K., DeCost, B., Chen, C., Jain, A., Tavazza, F., Cohn, R., Park, C. W., Choudhary, A., Agrawal, A., Billinge, S. J. L., Holm, E., Ong, S. P., & Wolverton, C. (2022). Recent advances and applications of deep learning methods in

- materials science. *Npj Computational Materials*, 8(1), 59. <https://doi.org/10.1038/s41524-022-00734-6>
- Choung, S., Kim, Y., Jang, M. G., Cho, G. H., Kang, D. G., Lee, T., Lee, D., Han, S., Seo, B., Park, W., Kim, M., Seo, O., Watanabe, T., Kumara, L. S. R., Matsumura, D., Kim, T. Y., Kim, J. H., Kim, J., & Han, J. W. (2026). Hierarchical ceria nanoarchitecture enabling accelerated lattice oxygen activation for efficient redox reactions. *Nature Communications*. <https://doi.org/10.1038/s41467-026-72447-z>
- Desimpel, S., Dorbec, M., Van Geem, K. M., & Stevens, C. V. (2026). Bayesian optimization for chemical reactions. *Chemical Society Reviews*, 55(5), 2731–2775. <https://doi.org/10.1039/D5CS00962F>
- Ganduglia-Pirovano, M. V., Hofmann, A., & Sauer, J. (2007). Oxygen vacancies in transition metal and rare earth oxides: Current state of understanding and remaining challenges. *Surface Science Reports*, 62(6), 219–270. <https://doi.org/10.1016/j.surfrep.2007.03.002>
- Hair, J. F., Black, W. C., Babin, B. J., & Anderson, R. E. (2019). *Multivariate Data Analysis*. Cengage. <https://books.google.com.mx/books?id=0R9ZswEACAAJ>
- Hao, X., Zhang, S., Xu, Y., Tang, L., Inoue, K., Saito, M., Ma, S., Chen, C., Xu, B., Adschiri, T., & Ikuhara, Y. (2021). Surfactant-mediated morphology evolution and self-assembly of cerium oxide nanocrystals for catalytic and supercapacitor applications. *Nanoscale*, 13(23), 10393–10401. <https://doi.org/10.1039/D1NR01746B>
- Himanen, L., Geurts, A., Foster, A. S., & Rinke, P. (2019). Data-Driven Materials Science: Status, Challenges, and Perspectives. *Advanced Science*, 6(21). <https://doi.org/10.1002/advs.201900808>
- Khan, M. M., Ansari, S. A., Pradhan, D., Han, D. H., Lee, J., & Cho, M. H. (2014). Defect-Induced Band Gap Narrowed CeO₂ Nanostructures for Visible Light Activities. *Industrial & Engineering Chemistry Research*, 53(23), 9754–9763. <https://doi.org/10.1021/ie500986n>
- Konsolakis, M., & Lykaki, M. (2021). Facet-Dependent Reactivity of Ceria Nanoparticles Exemplified by CeO₂-Based Transition Metal Catalysts: A Critical Review. *Catalysts*, 11(4), 452. <https://doi.org/10.3390/catal11040452>
- Kronenberg, K., Rave, H., Ghaffari-Tabrizi-Wizsy, N., Nyckees, D., Elinkmann, M., Freitak, D., Linsen, L., Gonzalez de Vega, R., & Clases, D. (2025). Exploring high-dimensional LA-ICP-TOFMS data with uniform manifold approximation and projection (UMAP). *Journal of Analytical Atomic Spectrometry*, 40(12), 3473–3484. <https://doi.org/10.1039/D5JA00215J>
- Li, J., Lu, G., Li, H., Wang, Y., Guo, Y., & Guo, Y. (2011). Facile synthesis of 3D flowerlike CeO₂ microspheres under mild condition with high catalytic performance for CO oxidation. *Journal of Colloid and Interface Science*, 360(1), 93–99. <https://doi.org/10.1016/j.jcis.2011.04.052>
- Li, Z.-X., Li, L.-L., Yuan, Q., Feng, W., Xu, J., Sun, L.-D., Song, W.-G., & Yan, C.-H. (2008). Sustainable and Facile Route to Nearly Monodisperse Spherical Aggregates of CeO₂ Nanocrystals with Ionic Liquids and Their Catalytic Activities for CO Oxidation. *The Journal of Physical Chemistry C*, 112(47), 18405–18411. <https://doi.org/10.1021/jp807348n>
- Liu, X., Yang, H., Han, L., Liu, W., Zhang, C., Zhang, X., Wang, S., & Yang, Y. (2013). Mesoporous-shelled CeO₂ hollow nanospheres synthesized by a one-pot hydrothermal route and their catalytic performance. *CrystEngComm*, 15(38), 7769. <https://doi.org/10.1039/c3ce40959g>
- Lookman, T., Balachandran, P. V., Xue, D., & Yuan, R. (2019). Active learning in materials science with emphasis on adaptive sampling using uncertainties for targeted design. *Npj Computational Materials*, 5(1), 21. <https://doi.org/10.1038/s41524-019-0153-8>
- Mai, H.-X., Sun, L.-D., Zhang, Y.-W., Si, R., Feng, W., Zhang, H.-P., Liu, H.-C., & Yan, C.-H. (2005). Shape-Selective Synthesis and Oxygen Storage Behavior of Ceria Nanopolyhedra, Nanorods, and Nanocubes. *The Journal of Physical Chemistry B*, 109(51), 24380–24385. <https://doi.org/10.1021/jp055584b>
- McInnes, L., Healy, J., & Melville, J. (2020). UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction. *ArXiv Preprint ArXiv:1802.03426*. <http://arxiv.org/abs/1802.03426>
- Meher, S. K., & Ranga Rao, G. (2012). Tuning, via Counter Anions, the Morphology and Catalytic Activity of CeO₂ Prepared under Mild Conditions. *Journal of Colloid and Interface Science*, 373(1), 46–56. <https://doi.org/10.1016/j.jcis.2011.09.050>
- Montini, T., Melchionna, M., Monai, M., & Fornasiero, P. (2016). Fundamentals and Catalytic Applications of CeO₂-Based Materials. *Chemical Reviews*, 116(10), 5987–6041. <https://doi.org/10.1021/acs.chemrev.5b00603>
- Nguyen, T.-D., Dinh, C.-T., Mrabet, D., Tran-Thi, M.-N., & Do, T.-O. (2013). Controlled synthesis of ceria nanoparticles for the design of nanohybrids. *Journal of Colloid and Interface Science*, 394, 100–107. <https://doi.org/10.1016/j.jcis.2012.12.020>
- Nolan, M., Parker, S. C., & Watson, G. W. (2005). The electronic structure of oxygen vacancy defects at the low index surfaces of ceria. *Surface Science*, 595(1–3), 223–232. <https://doi.org/10.1016/j.susc.2005.08.015>
- Parsaeifard, B., Sankar De, D., Christensen, A. S., Faber, F. A., Kocer, E., De, S., Behler, J., Anatole von Lilienfeld, O., & Goedecker, S. (2021). An assessment of the structural resolution of various fingerprints commonly used in machine learning. *Machine Learning: Science and Technology*, 2(1), 015018. <https://doi.org/10.1088/2632-2153/abb212>
- Pyzer-Knapp, E. O., Pitera, J. W., Staar, P. W. J., Takeda, S., Laino, T., Sanders, D. P., Sexton, J., Smith, J. R., & Curioni, A. (2022). Accelerating materials discovery using artificial intelligence, high performance computing and robotics. *Npj*

- Computational Materials*, 8(1), 84. <https://doi.org/10.1038/s41524-022-00765-z>
- Rajan, K. (2015). Materials Informatics: The Materials “Gene” and Big Data. *Annual Review of Materials Research*, 45(1), 153–169. <https://doi.org/10.1146/annurev-matsci-070214-021132>
- Shan, W., Guo, H., Liu, C., & Wang, X. (2012). Controllable preparation of CeO₂ nanostructure materials and their catalytic activity. *Journal of Rare Earths*, 30(7), 665–669. [https://doi.org/10.1016/S1002-0721\(12\)60109-4](https://doi.org/10.1016/S1002-0721(12)60109-4)
- Snoek, J., Larochelle, H., & Adams, R. P. (2012). Practical Bayesian Optimization of Machine Learning Algorithms. *Advances in Neural Information Processing Systems*, 4, 2951–2959. <http://arxiv.org/abs/1206.2944>
- Sun, C., Li, H., Zhang, H., Wang, Z., & Chen, L. (2005). Controlled synthesis of CeO₂ nanorods by a solvothermal method. *Nanotechnology*, 16(9), 1454–1463. <https://doi.org/10.1088/0957-4484/16/9/006>
- Szymanski, N. J., Rendy, B., Fei, Y., Kumar, R. E., He, T., Milsted, D., McDermott, M. J., Gallant, M., Cubuk, E. D., Merchant, A., Kim, H., Jain, A., Bartel, C. J., Persson, K., Zeng, Y., & Ceder, G. (2023). An autonomous laboratory for the accelerated synthesis of inorganic materials. *Nature*, 624(7990), 86–91. <https://doi.org/10.1038/s41586-023-06734-w>
- Tian, J., Zhong, J., Xie, Z., Cai, H., Song, L., Lei, K., Zhong, X., Liu, P., Shang, S., Ren, Q., Huang, H., Chen, L., Fu, M., & Ye, D. (2026). Activating lattice oxygen via self-adaptive Ce⁴⁺–O–Ce³⁺ symmetry-breaking sites in ceria for volatile organic compounds oxidation. *Applied Catalysis B: Environment and Energy*, 385, 126307. <https://doi.org/10.1016/j.apcatb.2025.126307>
- Trovarelli, A. (1996). Catalytic Properties of Ceria and CeO₂ - Containing Materials. *Catalysis Reviews*, 38(4), 439–520. <https://doi.org/10.1080/01614949608006464>
- Ulugöl, A., Bückmann, J., Yang, R., Hoitink, R., van Blaaderen, A., Smalenburg, F., & Filion, L. (2025). *Comparing unsupervised learning methods for local structural identification in colloidal systems*. <http://arxiv.org/abs/2509.07186>
- Urbach, F. (1953). The Long-Wavelength Edge of Photographic Sensitivity and of the Electronic Absorption of Solids. *Physical Review*, 92(5), 1324–1324. <https://doi.org/10.1103/PhysRev.92.1324>
- Wang, X., Jiang, Z., Zheng, B., Xie, Z., & Zheng, L. (2012). Synthesis and shape-dependent catalytic properties of CeO₂ nanocubes and truncated octahedra. *CrystEngComm*, 14(22), 7579. <https://doi.org/10.1039/c2ce25333j>
- Yang, C., Yu, X., Heißler, S., Nefedov, A., Colussi, S., Llorca, J., Trovarelli, A., Wang, Y., & Wöll, C. (2017). Surface Faceting and Reconstruction of Ceria Nanoparticles. *Angewandte Chemie International Edition*, 56(1), 375–379. <https://doi.org/10.1002/anie.201609179>
- Yang, S., & Gao, L. (2006). Controlled Synthesis and Self-Assembly of CeO₂ Nanocubes. *Journal of the American Chemical Society*, 128(29), 9330–9331. <https://doi.org/10.1021/ja063359h>
- Yao, H., Wang, Y., Jing, Y., & Luo, G. (2018). Ultrafast, Continuous and Shape-Controlled Preparation of CeO₂ Nanostructures: Nanorods and Nanocubes in a Microfluidic System. *Industrial & Engineering Chemistry Research*, 57(22), 7525–7532. <https://doi.org/10.1021/acs.iecr.8b01298>
- Zhang, D., Du, X., Shi, L., & Gao, R. (2012). Shape-controlled synthesis and catalytic application of ceria nanomaterials. *Dalton Transactions*, 41(48), 14455. <https://doi.org/10.1039/c2dt31759a>
- Zhou, K., Wang, X., Sun, X., Peng, Q., & Li, Y. (2005). Enhanced catalytic activity of ceria nanorods from well-defined reactive crystal planes. *Journal of Catalysis*, 229(1), 206–212. <https://doi.org/10.1016/j.jcat.2004.11.004>