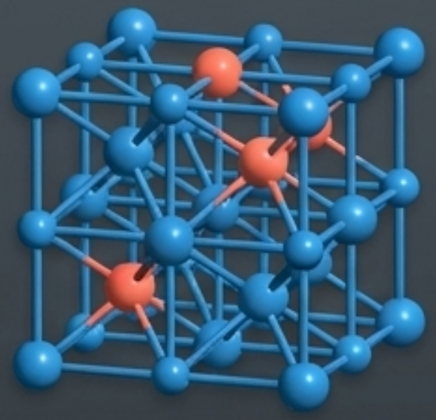
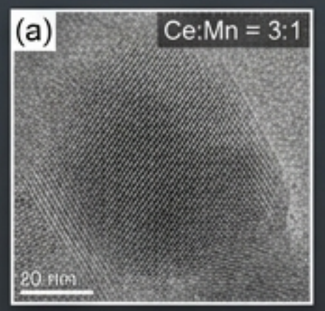
Composition dictates the structural fate of Mn-Ce mixed oxides



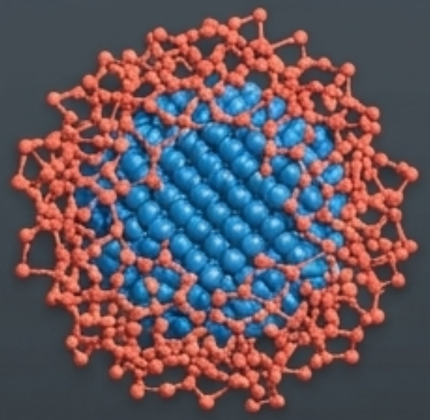


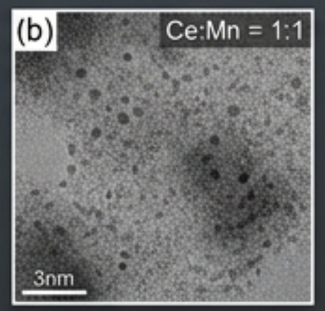
Solid Solution (Low Mn, x ≤ 0.25)

Structural State: Single-phase cubic fluorite solid solution.

Thermodynamics: Conforms to Vegard's law. Lattice contraction and localized strain occur due to smaller ionic radius of Mn vs host Ce.

Catalytic Profile: High bulk oxygen mobility but lower surface area.



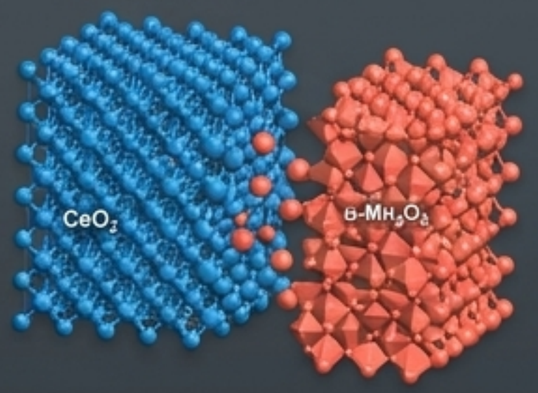


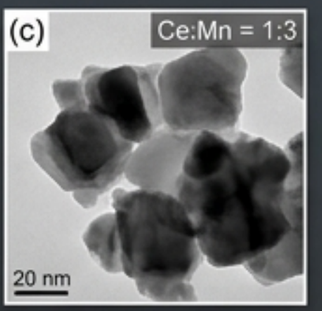
Ultrafine High-Activity (Ce:Mn = 1:1)

Structural State: Solubility limit reached. Metastable solid solution with amorphous MnO_x surface phase.

Thermodynamics: Maximum oxygen vacancy concentration. High Ce^{3+} defect density.

Catalytic Profile: Peak activity. Rapid lattice oxygen exchange via Mars-van Krevelen loops.





Phase Separation (High Mn, x > 0.50)

Structural State: Bulk crystalline precipitation (α-Mn_2O_3, Mn_3O_4).

Thermodynamics: Thermodynamically unstable solid solution upon calcination.

Catalytic Profile: Reduced activity. Loss of interfacial Mn–O–Ce synergistic bonds.

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The NanoLatticAI simulation engine translates physical parameters into predictive metrics

Input Process Parameters

Thermodynamic Levers

Temp_Target	550.0
Temp_Final	300.0
Pressure_atm	0.05

Chemical Levers

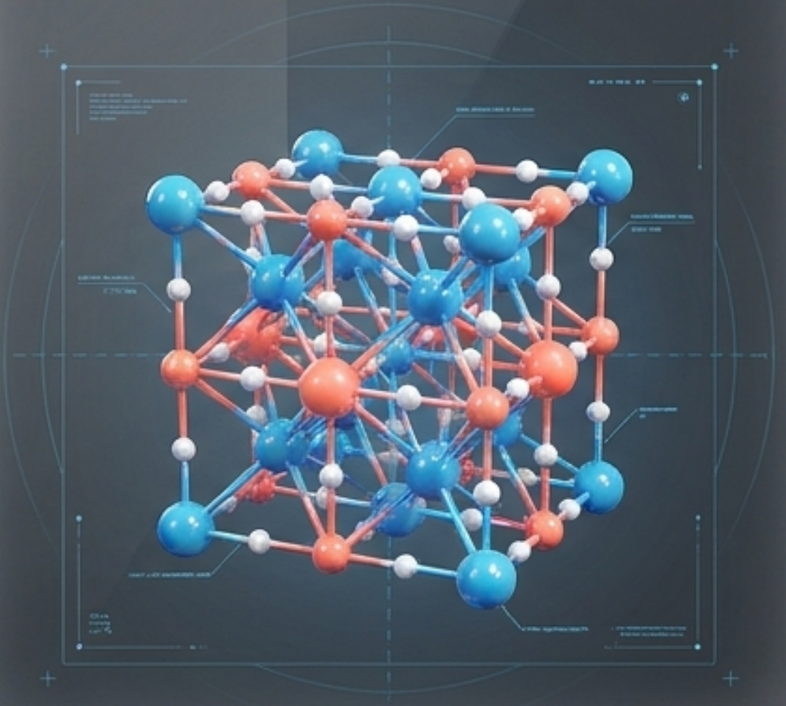
O_Metal_Ratio	1.8
Mn_Fraction	0.3
pH_Charge_Scale	8.5

Kinetic Levers

Heat_Steps	25000
Cool_Steps	3000
Shear_Rate	1.5

Black Box

Molecular Dynamics Engine for Ce-Mn-O



Output Telemetry

Morphology Targets

Y2_Size_Rg	18.72
Y3_Num_Clusters	6342
Y4_Compactness	-800.9

Thermodynamic States

Y1_Energy	-234.46
Y8_Worst_Defect_Energy	-0.18

Macro-Structure

Y10_Aggregation_Ratio	24.57
Y11_Phase_Sep_Dist	7.81
Y12_Core_Shell_Ratio	-3.32

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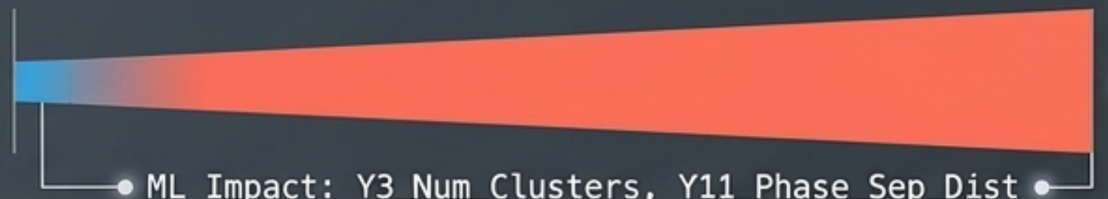
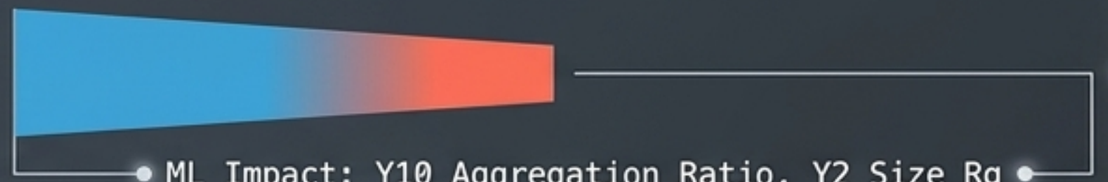
SHAP feature importance reveals O_Metal_Ratio as the dominant morphological driver

O_Metal_Ratio



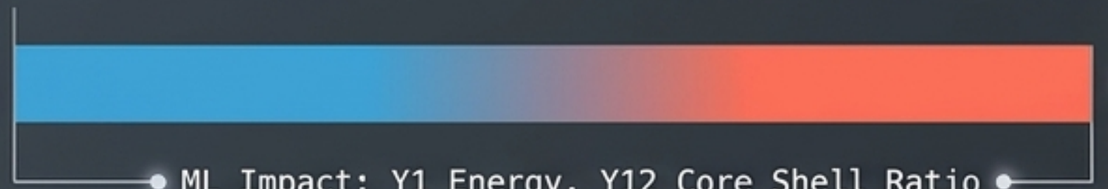
Physical Intuition: Oxygen-to-metal stoichiometry acts as the master switch. Forcing an oxygen-deficient ratio artificially lowers the formation energy of oxygen vacancies, accelerating the segregation of MnOx phases and cluster formation.

Target_Box_Size



Physical Intuition: Defines the spatial constraints of the simulation volume, closely mirroring the physical kinetics of particle aggregation and shear rate boundaries in hydrothermal synthesis.

Temp_Target



Physical Intuition: Dictates thermodynamic mobility. Elevated temperatures force the transition from metastable solid solutions toward core-shell stratification to minimize surface energy.

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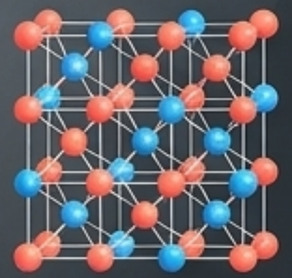
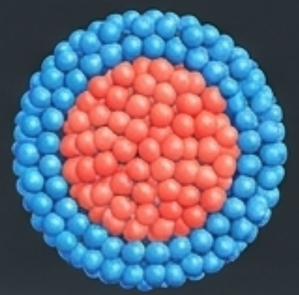
The **Morphology Blueprint:** Parameter sets for targeted catalytic architecture

Target State	Stoichiometry	NanoLatticAI Optimization	Catalytic Advantage
 Solid Solution Matrix	Low Mn (x ≤ 0.25)	Maximize Temp_Target, minimize O_Metal_Ratio	Superior bulk oxygen transport. Ideal for steady-state, high-temperature environmental remediation.
 Ultrafine High-Activity (2-4 nm)	Equimolar (Ce:Mn = 1:1)	Balance Shear_Rate, minimize Target_Box_Size to restrict growth, tune O_Metal_Ratio for max Y3_Num_Clusters	Generates highest concentration of coordinatively unsaturated sites. Enables low-temperature CO/VOC oxidation.
 Core-Shell Architecture	Variable (Template dependent)	Rapid Cool_Steps to induce kinetic trapping, maximizing Y12_Core_Shell_Ratio while suppressing Y11_Phase_Sep_Dist	Defensive Engineering. Outer shell shields inner active manganese sites from direct chemical sulfation, mitigating SO2 poisoning.

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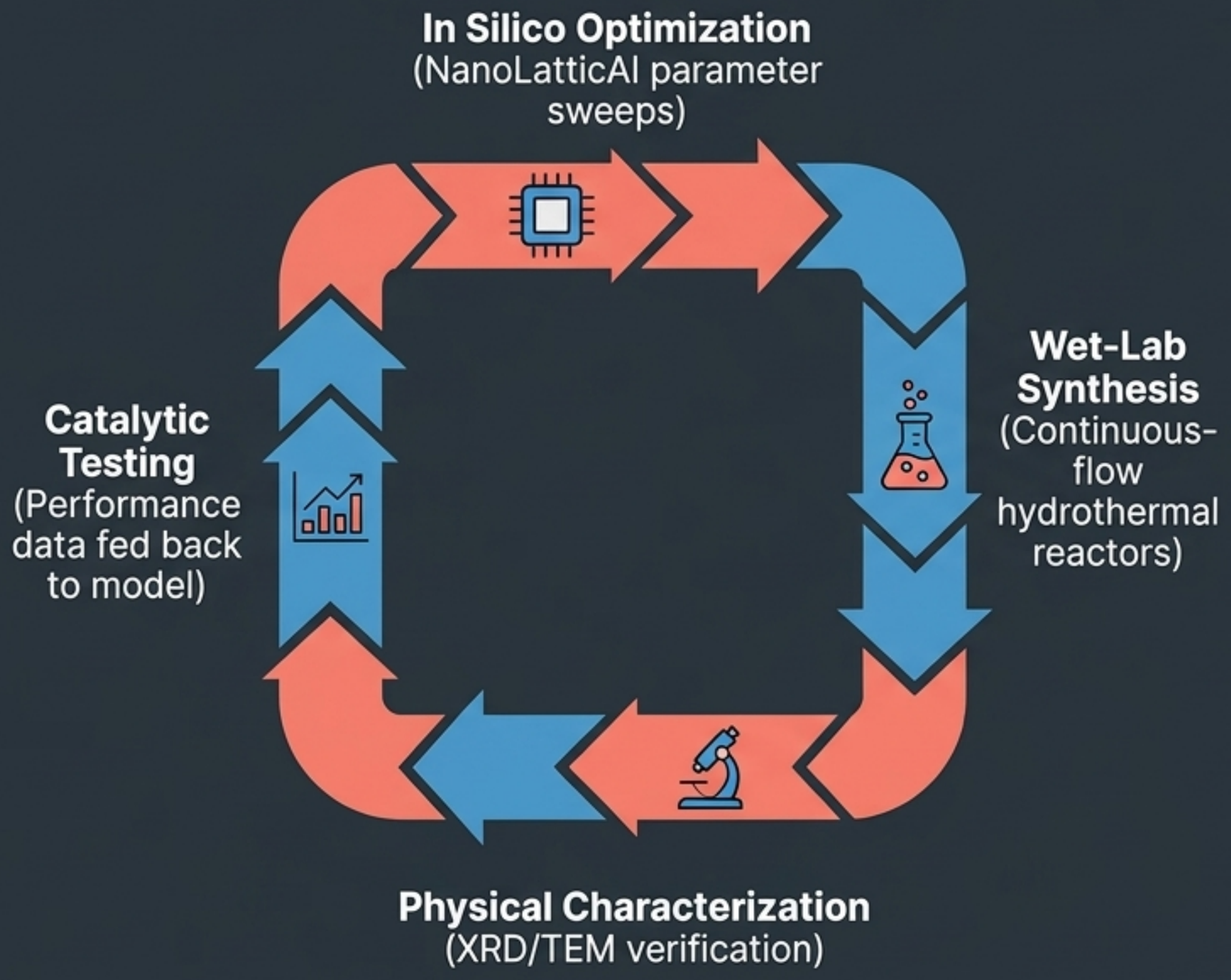
Integrating ***in silico*** prediction with physical synthesis pipelines



Key Strategic Takeaways

01 / The Equimolar Synergistic Peak

Maintaining a near 1:1 ratio avoids bulk crystalline phase separation while maximizing the active amorphous MnOx surface phase.

02 / Oxygen Control is Structural Control

The `O_Metal_Ratio` is the dominant simulator dial; tuning it accurately predicts real-world defect concentrations and cluster behaviors.

03 / Programmable Durability

Simulated core-shell topologies offer a direct pathway to solving industrial sulfur poisoning, enabling long-term deployment in harsh environments.

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