

Structure sensitivity of $\text{La}_2\text{O}_2\text{CO}_3$ catalysts in the oxidative coupling of methane

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Table S1 The calculated density of sites for O₂ and CO₂ adsorption over different samples based on TPD data.

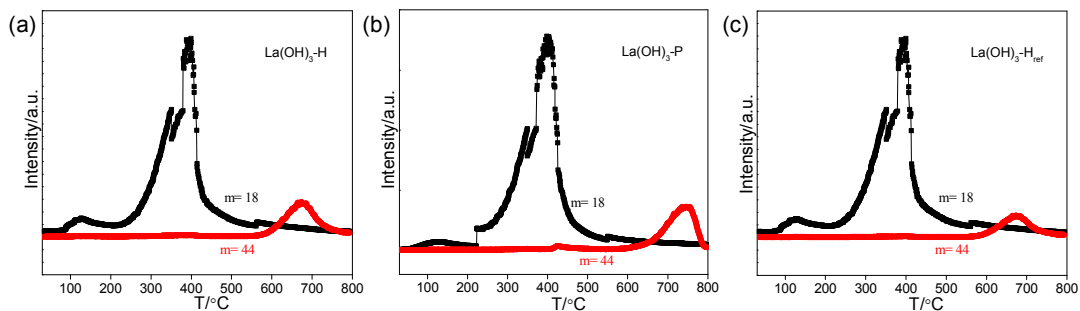
Samples	$\rho_{\text{O}_2}/\mu\text{mol}\cdot\text{m}^{-2}$		$\rho_{\text{CO}_2}/\mu\text{mol}\cdot\text{m}^{-2}$	
	T=200-400 °C	T=400-600 °C	T=400-600 °C	T=600-800 °C
La ₂ O ₂ CO ₃ -H	0.52	0.86	1.24	4.07
La ₂ O ₂ CO ₃ -P	0.03	-	0.24	9.02
La ₂ O ₂ CO ₃ -H _{ref}	-	-	-	3.49
La ₂ O ₃ -H	-	0.11	-	7.41
La ₂ O ₃ -P	-	-	-	11.90
La ₂ O ₃ -H _{ref}	-	-	-	7.00

Table S2 Areas of the oxygen species peaks based on O 1s binding energy spectra of the La₂O₂CO₃ samples and the ratio of (O⁻+O₂²⁻)/O²⁻.

Samples	Binding energy/eV				(O ⁻ +O ₂ ²⁻)/O ²⁻
	528.2 (O ²⁻)	530.1 (O ⁻)	531.1 (O ₂ ²⁻)	532.2 (CO ₃ ²⁻)	
La ₂ O ₂ CO ₃ -H	10156.3	15260.8	50590.7	31589.6	6.5
La ₂ O ₂ CO ₃ -P	9983.7	5844.7	30738.9	4460.4	3.7
La ₂ O ₂ CO ₃ -H _{ref}	14290.0	17651.8	35834.2	3153.6	3.7

Table S3 The calculated surface atomic composition of the La₂O₂CO₃ samples based on XPS analysis.

Samples	Atomic composition/%		
	O	La	C
La ₂ O ₂ CO ₃ -H	55.5	18.2	26.3
La ₂ O ₂ CO ₃ -P	57.5	18.6	23.9
La ₂ O ₂ CO ₃ -H _{ref}	61.0	16.5	22.5

**Figure S1** TPD-MS traces for H₂O and CO₂ corresponding to the thermal decomposition of samples (a) La(OH)₃-H, (b) La(OH)₃-P and (c) La(OH)₃-H_{ref} in air.

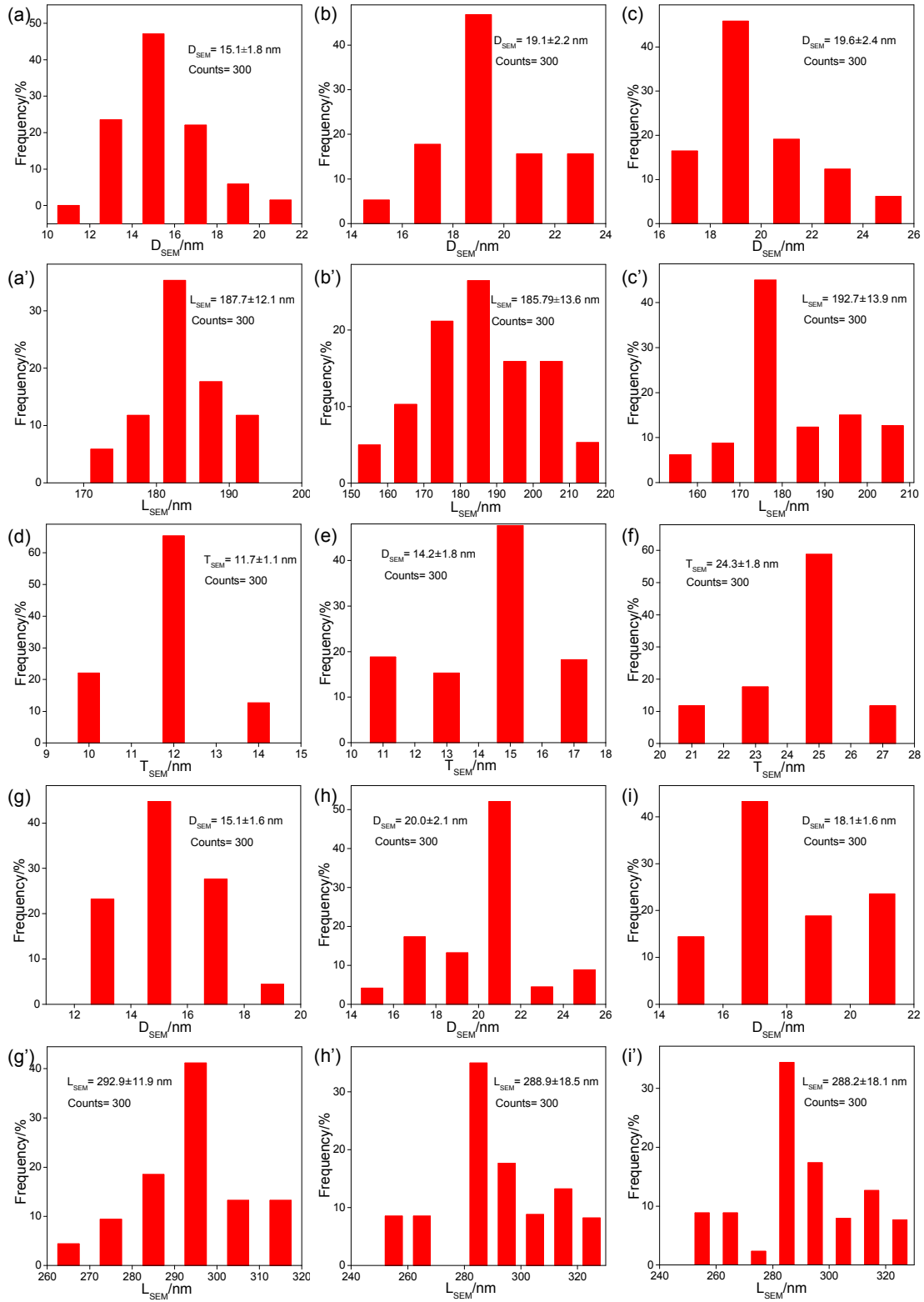


Figure S2 Particle sizes distribution of samples (a, a') $La(OH)_3-H$, (b, b') $La_2O_2CO_3-H$, (c, c') La_2O_3-H , (d) $La(OH)_3-P$, (e) $La_2O_2CO_3-P$, (f) La_2O_3-P , (g, g') $La(OH)_3-H_{ref}$, (h, h') $La_2O_2CO_3-H_{ref}$, and (i, i') $La_2O_3-H_{ref}$. D_{SEM} , L_{SEM} , and T_{SEM} stand for diameters, length, and thickness of the samples, respectively.

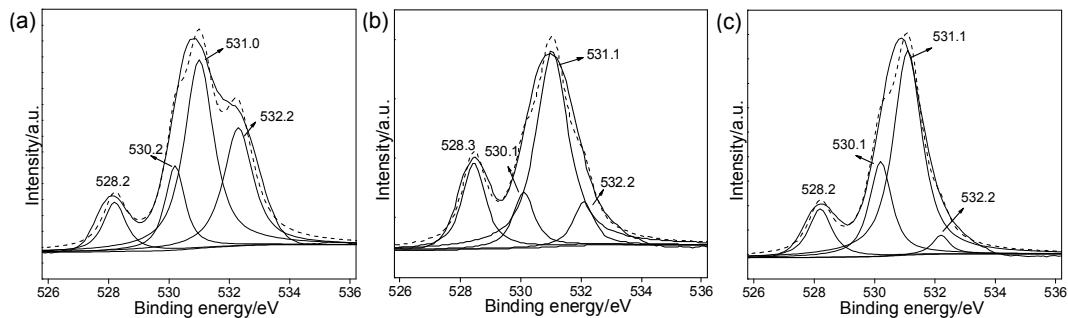


Figure S3 O 1s binding energy spectra of the samples (a) $\text{La}_2\text{O}_2\text{CO}_3\text{-H}$, (b) $\text{La}_2\text{O}_2\text{CO}_3\text{-P}$, and (c) $\text{La}_2\text{O}_2\text{CO}_3\text{-H}_{\text{ref}}$.

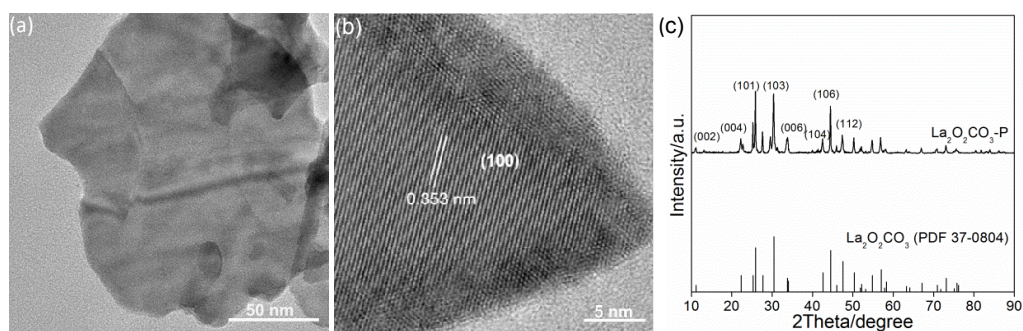


Figure S4. TEM, HRTEM images and XRD patterns of the sample $\text{La}_2\text{O}_2\text{CO}_3\text{-P}$.

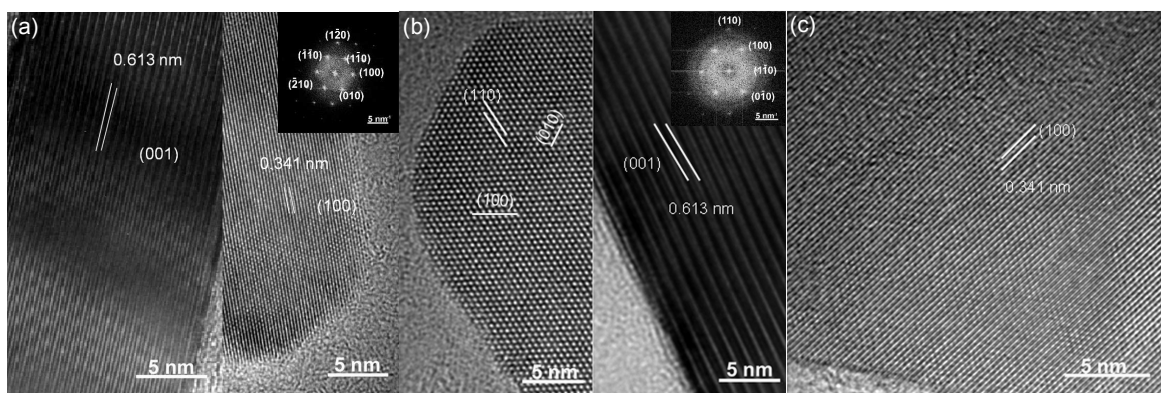


Figure S5 HRTEM images, SAED patterns of the samples $\text{La}_2\text{O}_3\text{-H}$ (a) and $\text{La}_2\text{O}_3\text{-H}_{\text{ref}}$ (b), and HRTEM images of the sample $\text{La}_2\text{O}_3\text{-P}$ (c).

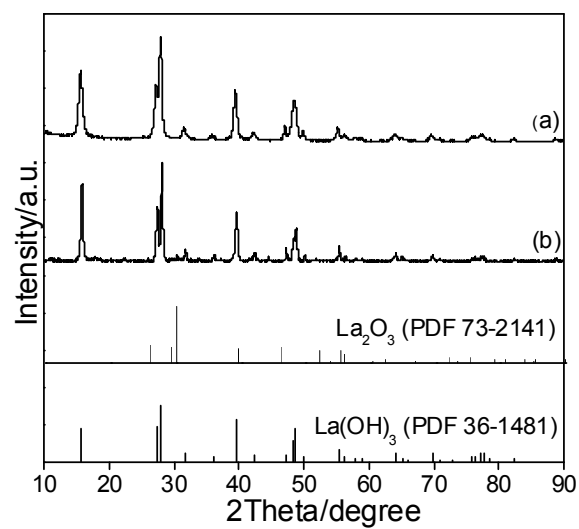


Figure S6 XRD patterns of the fresh sample $\text{La}(\text{OH})_3\text{-H}$ (a) and the hydrolysis-treated sample $\text{La}_2\text{O}_3\text{-H}$ (b).

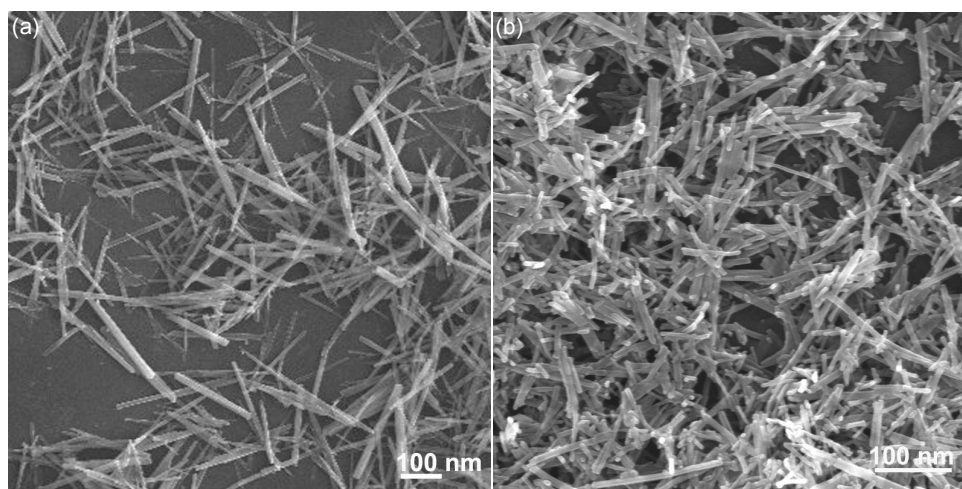


Figure S7 SEM images of the fresh sample $\text{La}(\text{OH})_3\text{-H}$ (a) and the hydrolysis-treated sample $\text{La}_2\text{O}_3\text{-H}$ (b).