

## ***Electronic Supplementary Information (ESI)***

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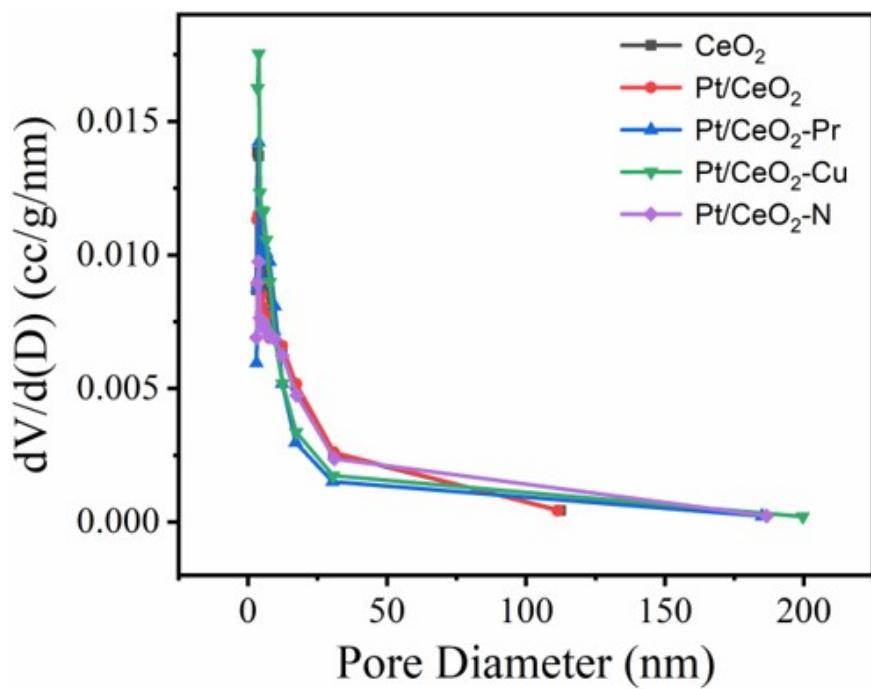
# **Fabrication of supported Pt/CeO<sub>2</sub> nanocatalysts doped with different elements for CO oxidation: Theoretical and experimental studies**

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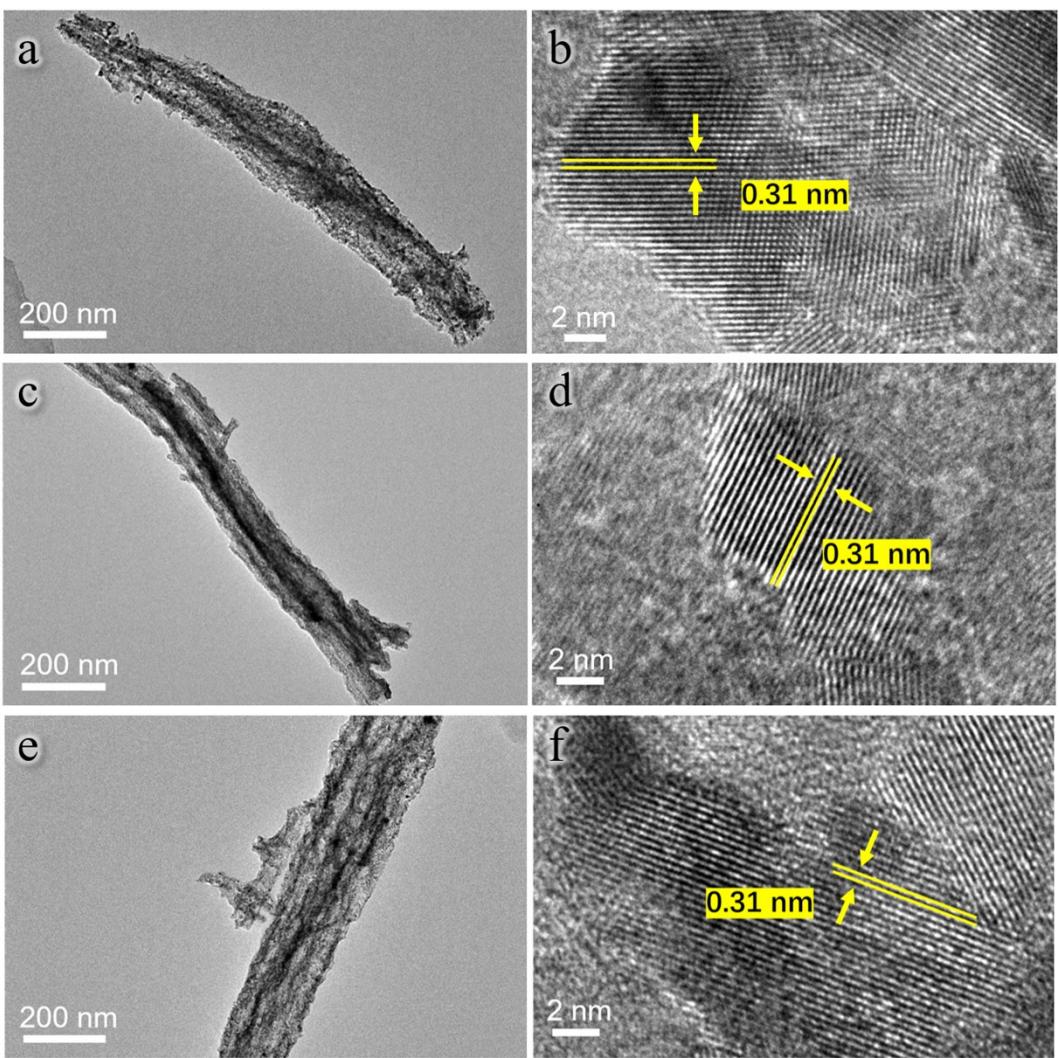
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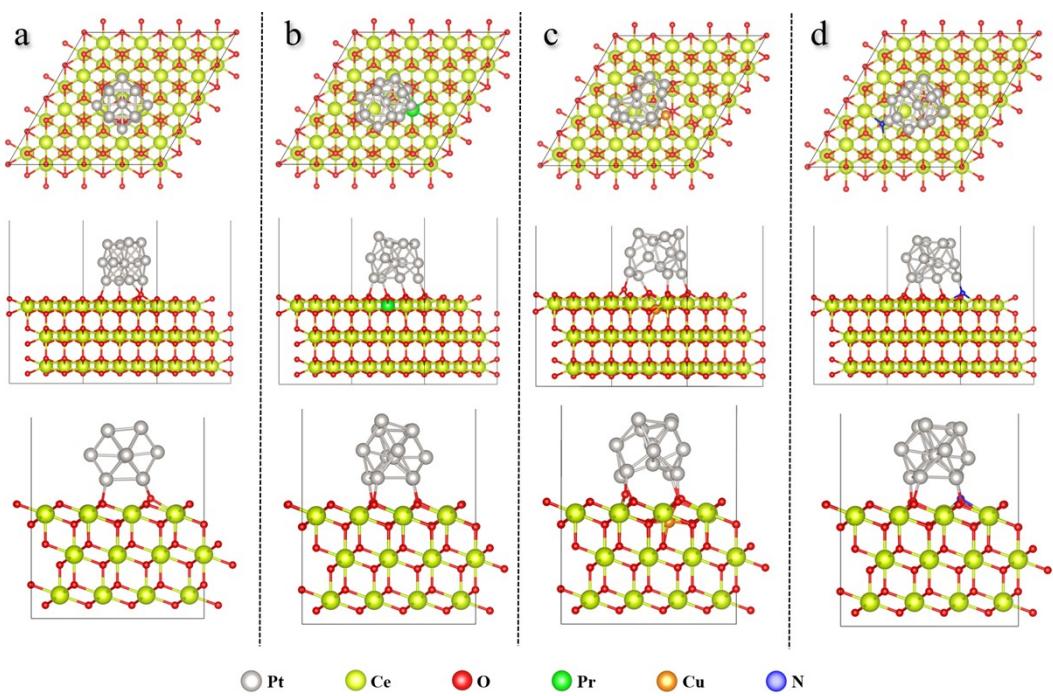
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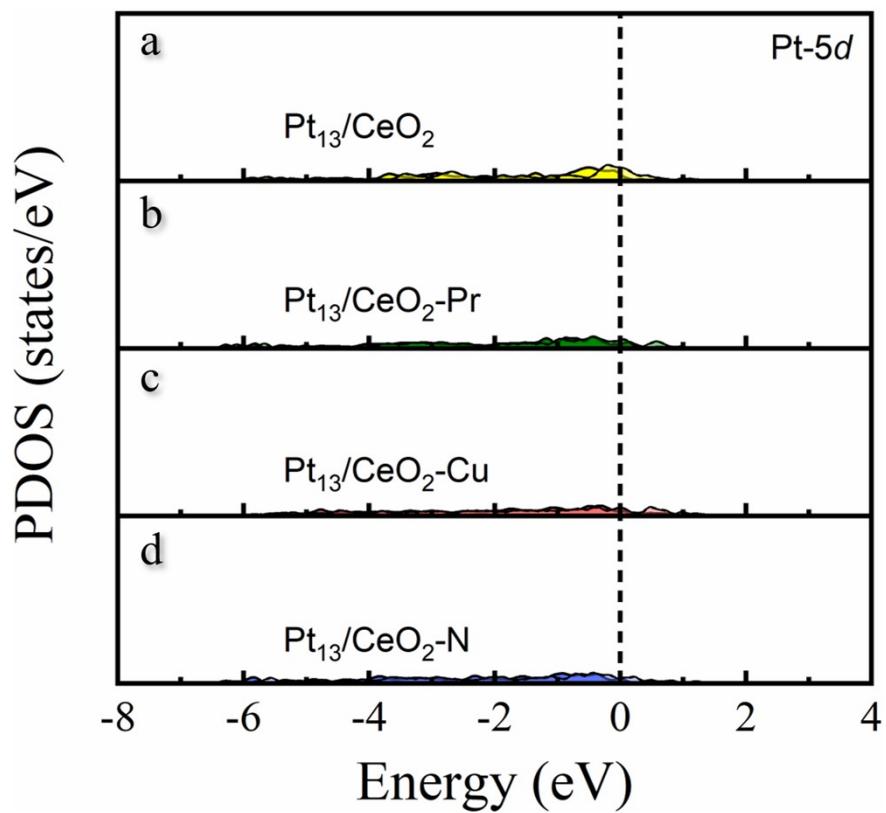
**Figure S1.** Pore size distribution plots of  $\text{CeO}_2$ ,  $\text{Pt}/\text{CeO}_2$ , and  $\text{Pt}/\text{CeO}_2\text{-M}$  ( $\text{M} = \text{Pr}, \text{Cu}, \text{N}$ ).



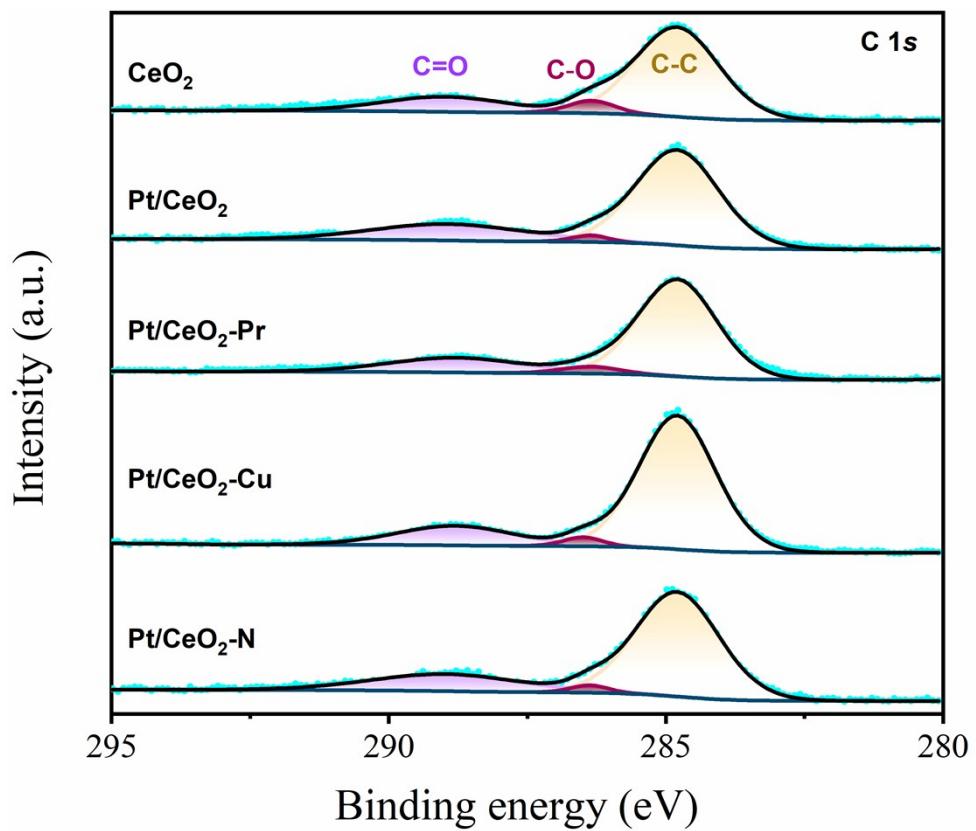
**Figure S2.** TEM and high-resolutionTEM images of (a, b) Pt/CeO<sub>2</sub>, (c, d) Pt/CeO<sub>2</sub>-Pr, and (e, f) Pt/CeO<sub>2</sub>-N samples.



**Figure S3.** The optimized models of the four catalysts (a)  $\text{Pt}_{13}/\text{CeO}_2$ , (b)  $\text{Pt}_{13}/\text{CeO}_2\text{-Pr}$ , (c)  $\text{Pt}_{13}/\text{CeO}_2\text{-Cu}$ , and (d)  $\text{Pt}_{13}/\text{CeO}_2\text{-N}$ .



**Figure S4.** PDOS of Pt-5d state of (a)  $\text{Pt}_{13}/\text{CeO}_2$ , (b)  $\text{Pt}_{13}/\text{CeO}_2\text{-Pr}$ , (c)  $\text{Pt}_{13}/\text{CeO}_2\text{-Cu}$ , and (d)  $\text{Pt}_{13}/\text{CeO}_2\text{-N}$ .



**Figure S5.** High-resolution XPS spectra of C 1s over five different catalysts.

**Table S1.** The activation energies ( $E_a$ ) of different catalysts reported in the literature.

Catalyst	Activation energies ( $E_a$ ) (kJ/mol)	Reference
$\text{CeO}_2$	64	[1]
$\text{FePc}/\text{CeO}_2$	50	[1]
$\text{Au}/\text{CeO}_2$	42	[1]
hemin/ $\text{CeO}_2$	61	[1]
hemin-Au/ $\text{CeO}_2$	21	[1]
$\text{FePc-Au}/\text{CeO}_2$	34	[1]
$\text{Pt/bio-CeO}_2$	45	[2]
$\text{Pd/bio-CeO}_2$	47	[2]
$\text{Au/bio-CeO}_2$	37	[2]
$\text{Ag/bio-CeO}_2$	49	[2]
$\text{Pt/CeO}_2$ 500C	55	[3]
$\text{Pt/CeO}_2$ 800C	79	[3]
$\text{Pt/(800C)CeO}_2$ 500C	33	[3]
$\text{Pt/(800C)CeO}_2$ 800C	56	[3]

## References

1. L. Fan, J. Dai, Z. Huang, J. Xiao, Q. Li, J. Huang, S.-F. Zhou and G. Zhan, *iScience*, 2020, **23**, 101852.
2. B. Jiang, X. Cha, Z. Huang, S. Hu, K. Xu, D. Cai, J. Xiao and G. Zhan, *Molecular Catalysis*, 2022, **524**, 112251.
3. J. Lee, Y. Ryou, J. Kim, X. Chan, T. J. Kim and D. H. Kim, *The Journal of Physical Chemistry C*, 2018, **122**, 4972-4983.