

Supporting Information

Trace Amount of Cu(OAc)₂ Boosting Efficiency on the Cumene Oxidation Catalyzed by Carbon Nanotubes Washed with HCl

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1. Supplemental Tables

Table S1 The content of metal impurities in pCNTs from ICP-AAS test.

Metal impurity	Content (ppm)
Fe	4268
Ni	0
Co	0
Zn	0
Mg	0
Ca	0

Table S2 Quantitative XPS analysis of the catalysts

Sample	Elemental distribution (at.%)		
	C	O	Cl
pCNTs	98.9	1.1	-
CNTs	98.55	1.38	0.07
CNT1	97.61	2.39	-
CNT2	98.37	1.63	-
CNT3	97.58	2.35	0.07

Table S3 Cl element content of different carbon catalysts based on the X-Ray Fluorescence analysis.

Catalyst	Cl element content (%)
pCNTs	0
CNTs	0.039

Table S4 Catalytic performance in cumene oxidation catalyzed by pCNTs and CuCl₂.^[a]

Entry	Catalysts (mg)		Con. (%)
	pCNTs	CuCl ₂	Cumene
1	100	0.8	54.8
2	100	3.45	66.4

^[a] Reaction conditions: 10 mL cumene, 25 mL min⁻¹ O₂, 80 °C, 8 h.

Table S5 Cumene oxidation catalyzed by HBr treated CNTs.^[a]

Entry	Catalysts		Conversion (%)
	Br-CNTs (mg) ^[b]	Addition	Cumene
1	100	-	41.6
2	100	Cu(OAc) ₂ ^[c]	44.4

^[a] Reaction conditions: 10 mL cumene, 25 mL min⁻¹ O₂, 80 °C, 8 h. ^[b] Washed by HBr solution.

^[c] 0.01 mg.

2. Supplemental Figures

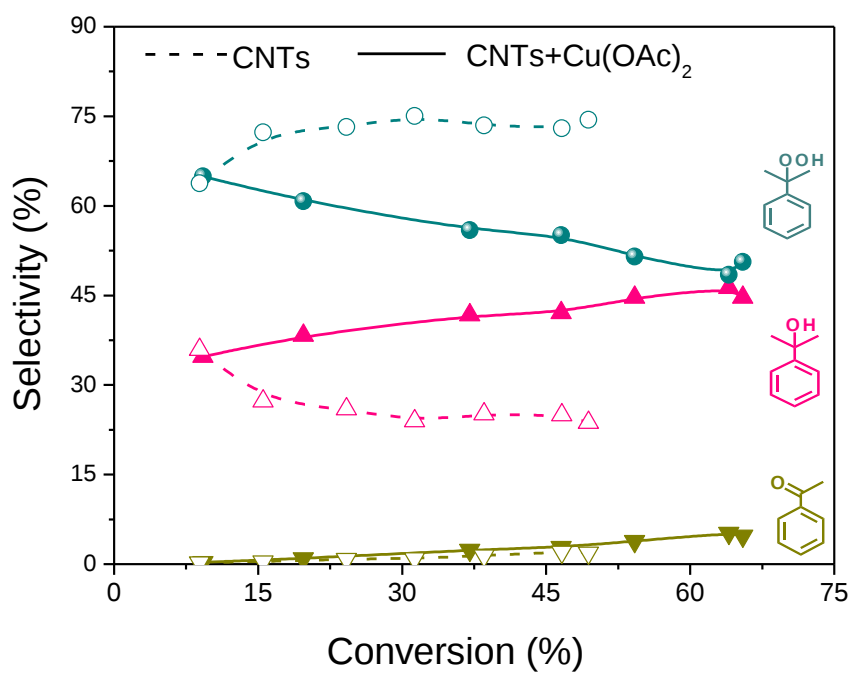


Figure S1 Cumene conversion *vs.* products selectivity distribution with and without $\text{Cu}(\text{OAc})_2$.

Reaction conditions: 10 mL cumene, 100 mg catalyst, 0.01 mg $\text{Cu}(\text{OAc})_2$ (if applicable), 25 mL/min O_2 , 80 °C.

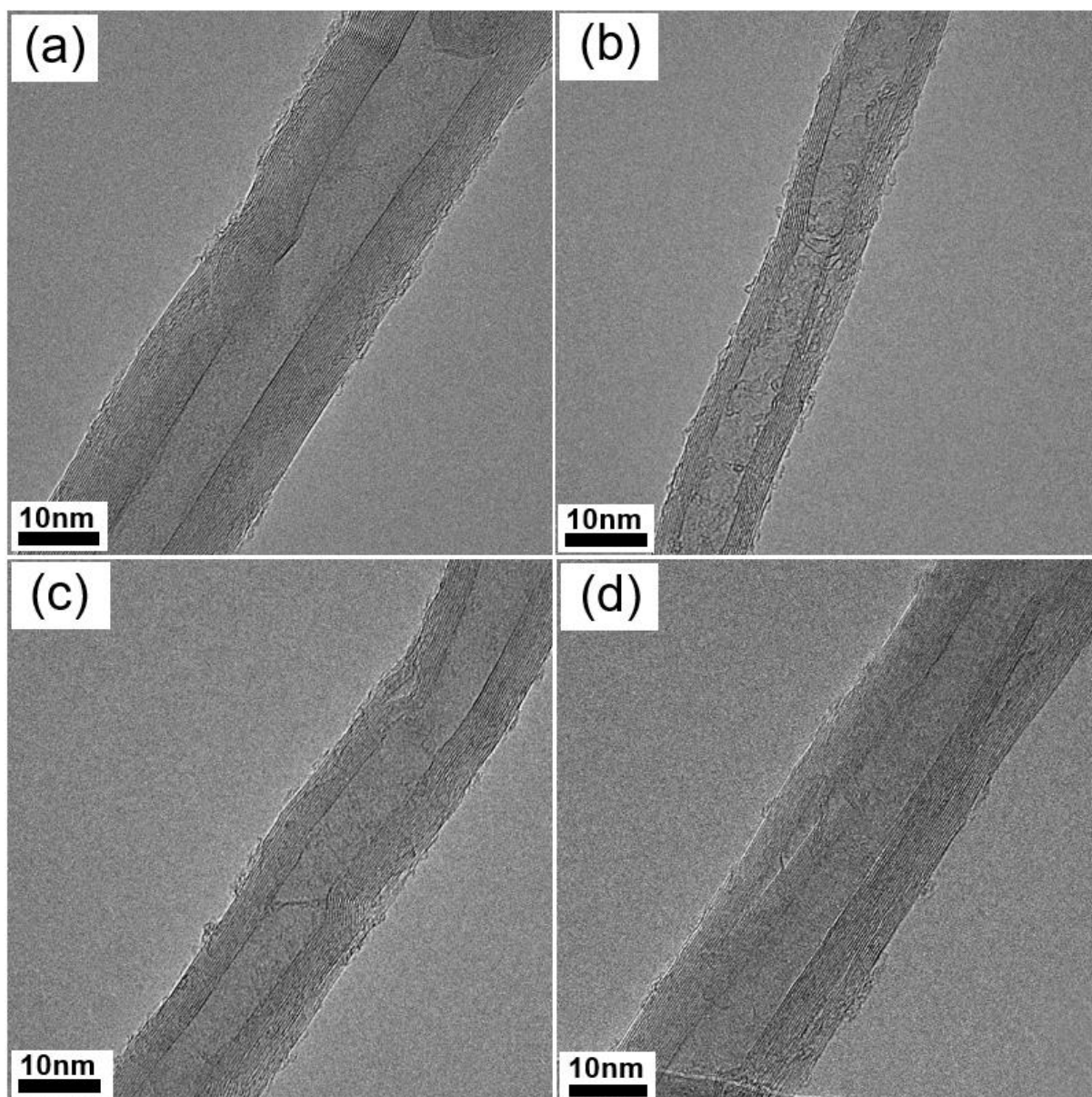


Figure S2 TEM images of CNTs (a), CNT1 (b), CNT2 (c), CNTs3 (d).

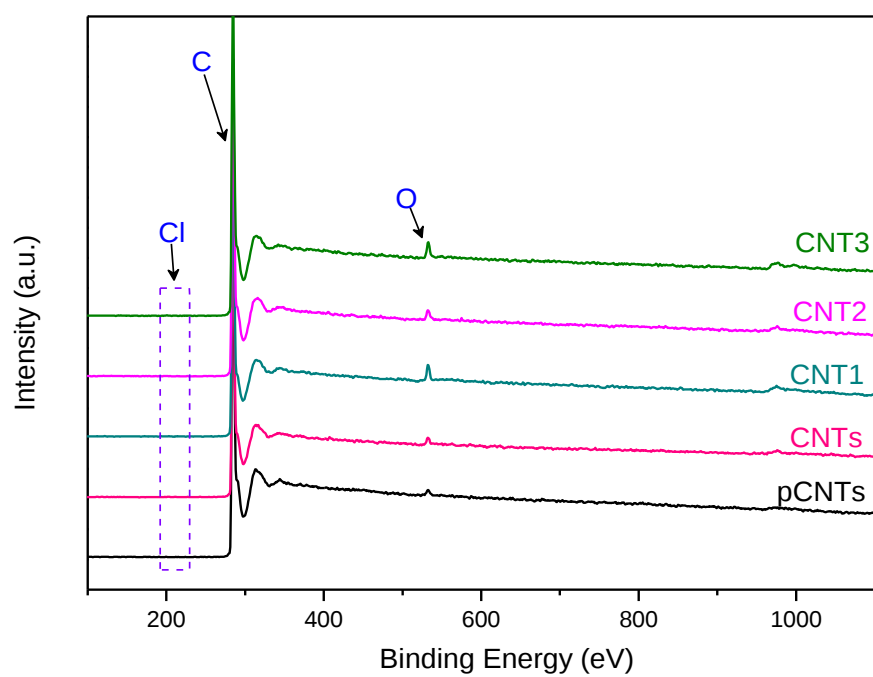


Figure S3 XPS survey of the catalysts.

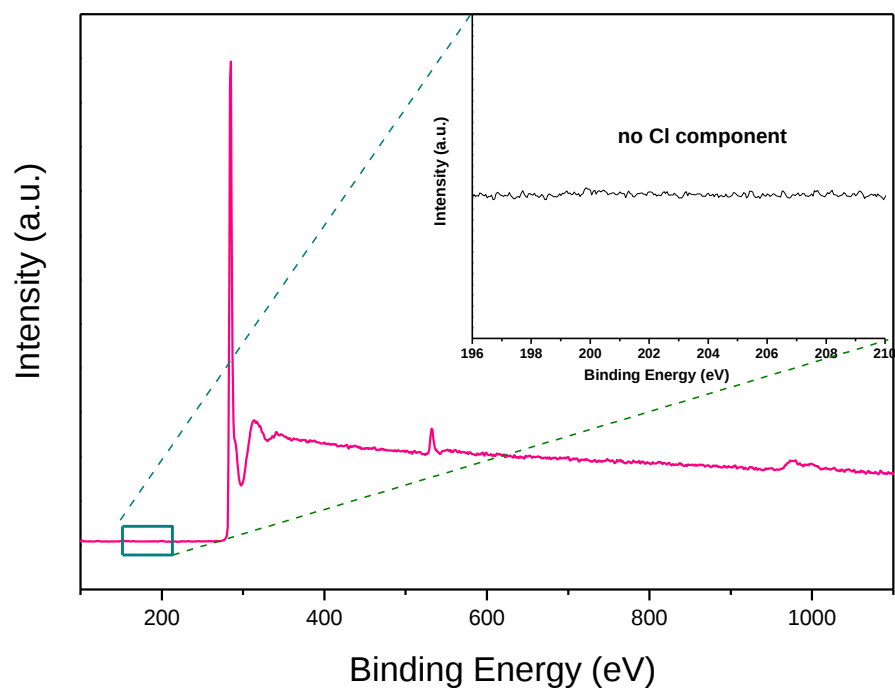


Figure S4 XPS survey and Cl detection of CNT4.

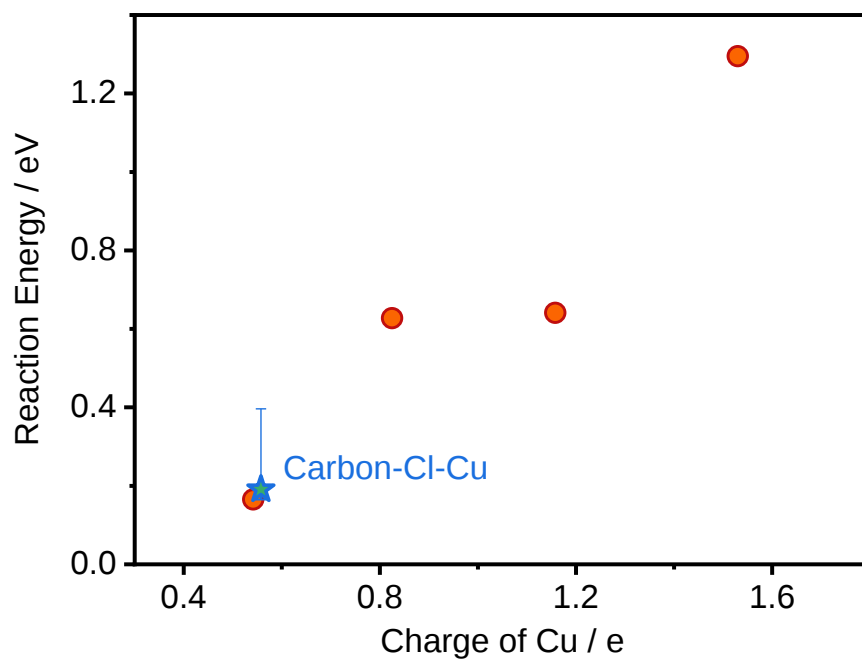


Figure S5 The correlation between the charge of Cu and reaction energy for the transformation from CHP to cumyl peroxy, corresponding to the upper part of Figure 3a in main text.

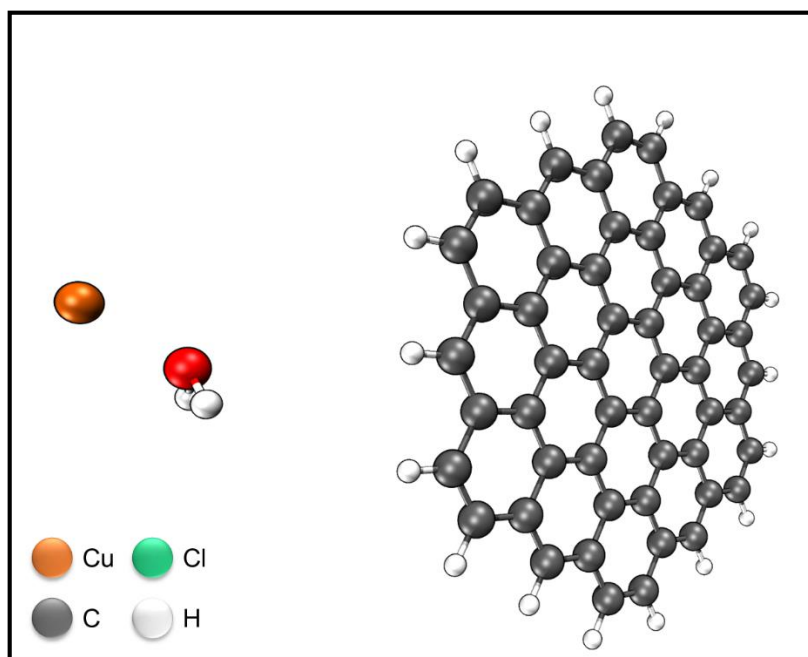


Figure S6 The interaction analysis based on independent gradient model (IGM) for carbon-H₂O-Cu. Isovalue is 0.003, comparing to Figure 3b in main text.