

Morphology Dependent, Green, and Selective Catalytic Styrene Oxidation on Co_3O_4

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Electronic Supplementary Information (ESI)

ESI 1. Calculation of turn-over frequency

Turn-over frequency (TOF) was calculated by using the measured conversion of 50 mg Co_3O_4 catalyst.

(a) Total no. of Co^{3+} site in 0.05gm of NR catalysts

Calculation of the total surface area of 0.05 g of Co_3O_4 NR

Volume of single NR(based on TEM)= $6 \times 6 \times 60 = 2160 \text{ nm}^3$

Density of $\text{Co}_3\text{O}_4 = 6.11 \text{ gm.cm}^{-3}$

Volume of 0.05 gm of $\text{Co}_3\text{O}_4 = 0.05 \text{ gm} / 6.11 \text{ gm.cm}^{-3} = 8.18 \times 10^{-3} \text{ cm}^3 = 8.18 \times 10^{18} \text{ nm}^3$

Total number of nanorods in 0.05 g of Co_3O_4 NRs = $V_{\text{total}} / V_{\text{each nanorod}} = 8.18 \times 10^{18} / 2160$
 $= 3.78 \times 10^{15}$

Total number of Co^{3+} ions on the surfaces of all Co_3O_4 nanorods: according to XPS analysis results Co_3O_4 NR contains almost 58% of Co^{3+} site at UHV RT. Hence.

Total no. of active site i.e. Co^{3+} sites in NR = $3.78 \times 10^{15} \times 58/100 = 2.19 \times 10^{15}$

(b) Total no. of Co^{3+} site in 0.05gm of NC catalysts

Calculation of the total surface area of 0.05 g of Co_3O_4 NC

Volume of single NC(based on TEM)= $20 \times 20 \times 20 = 8000 \text{ nm}^3$

Density of $\text{Co}_3\text{O}_4 = 6.11 \text{ gm.cm}^{-3}$

Volume of 0.05 gm of $\text{Co}_3\text{O}_4 = 0.05 \text{ gm} / 6.11 \text{ gm.cm}^{-3} = 8.18 \times 10^{-3} \text{ cm}^3 = 8.18 \times 10^{18} \text{ nm}^3$

Total number of nanorods in 0.05 g of Co_3O_4 NRs = $V_{\text{total}} / V_{\text{each nanorod}} = 8.18 \times 10^{18} / 8000$
 $= 1.02 \times 10^{15}$

Total number of Co^{3+} ions on the surfaces of all Co_3O_4 nanorods: according to XPS analysis results Co_3O_4 NR contains almost 60% of Co^{3+} site at UHV RT. Hence.

Total no. of Co^{3+} sites in NC catalyst = $1.02 \times 10^{15} \times 60/100 = 6.12 \times 10^{14}$

(c) Calculation of the total surface area of 0.05 g of Co_3O_4 HNR

Total no. of Co^{3+} site in 0.05gm of NC catalysts

Calculation of the total surface area of 0.05 g of Co_3O_4 NR

Volume of single HNR(based on TEM)= $10 \times 30 \times 120 = 36000 \text{ nm}^3$

Density of $\text{Co}_3\text{O}_4 = 6.11 \text{ gm.cm}^{-3}$

Volume of 0.05 gm of $\text{Co}_3\text{O}_4 = 0.05 \text{ gm} / 6.11 \text{ gm.cm}^{-3} = 8.18 \times 10^{-3} \text{ cm}^3 = 8.18 \times 10^{18} \text{ nm}^3$

Total number of nanorods in 0.05 g of Co_3O_4 NRs = $V_{\text{total}} / V_{\text{each nanorod}} = 8.18 \times 10^{18} / 36000$
 $= 2.27 \times 10^{14}$

Total number of Co³⁺ ions on the surfaces of all Co₃O₄ nanorods: according to XPS analysis results Co₃O₄ NR contains almost 50% of Co³⁺ site at UHV RT. Hence.

Total no. of Co³⁺ sites in 0.05 g of catalyst = $2.27 \times 10^{14} \times 50/100 = 1.13 \times 10^{14}$

(d) *No. of styrene molecules in 0.5 mmol of substrate* = $6.022 \times 10^{23} \times 0.5 \times 10^{-3}$

$$= 3.0 \times 10^{20}$$

TOF calculation = *no. of molecules(mole.) of reactant converted per active site of the catalyst/time*

Styrene (mmol)	Initial reactant taken(mole.)	Conversion (%)	Conversion (mole.)	No. of active sites	TON	TOF (sec ⁻¹)	TOF (min ⁻¹)	TOF (h ⁻¹)
0.5	0.3×10^{21}	100	0.3×10^{21}	1.02×10^{15}	2.9×10^5	16.1	966	5.79×10^4
5.0	3.1×10^{21}	49.8	1.5×10^{21}	1.02×10^{15}	14.7×10^5	81.6	4896	29.3×10^4
8.75	5.4×10^{21}	23.2	1.2×10^{21}	1.02×10^{15}	11.7×10^5	65	3900	23.4×10^4
13.1	8.1×10^{21}	17	1.4×10^{21}	1.02×10^{15}	13.7×10^5	76.1	4566	27.3×10^4
17.5	10.8×10^{21}	16	1.7×10^{21}	1.02×10^{15}	16.6×10^5	92.2	5532	33.2×10^4
26.5	16.4×10^{21}	7.3	1.2×10^{21}	1.02×10^{15}	11.7×10^5	65	3900	23.4×10^4