Supplementary Information

Zeolite imidazolate framework/g-C_3N_4 derived Co nanoparticles embedded in nitrogen doped carbon for efficient hydrogenation of phenol

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Table S1 Hydrogenation of phenol to cyclohexanol over various catalysts in references and this work

Catalysts	Reaction conditions				phenol	Cyclohexanol	Reference	Date
	T/°C	P/MPa	t/h	Solvent	Conversion/%	Selectivity/%		
Raney®Ni	220	2	2	water	87	52	[16]	2018
Ni/SiO_2	200	1	4	water	100	100	[17]	2017
Ni/NiCaAlO_x	110	2	3	n-hexane	99.9	99.9	[18]	2021
Co/CeO_2	150	3	16	water	82.5	100	[19]	2020
CoOx@C	150	3	16	water	98	77	[20]	2018
NiCo@C/ZrO_2	200	2	4	water	96	91	[21]	2019
NiCo/γ-Al_2O_3	250	2	4	water	82	85	[22]	2019
NiCo/SDSW	100	5	4	Isopropanol	99.9	99.9	[23]	2020
NiCo/Mg_xNi_yO	150	2	2.5	n-Hexane	99.9	99.9	[24]	2020
This work	120	2	3	water	97.8	100		

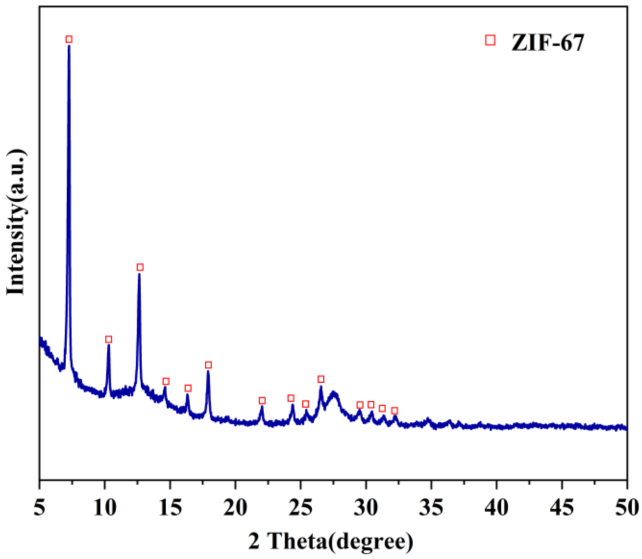


Fig. S1 XRD pattern of ZIF-67/g-C_3N_4

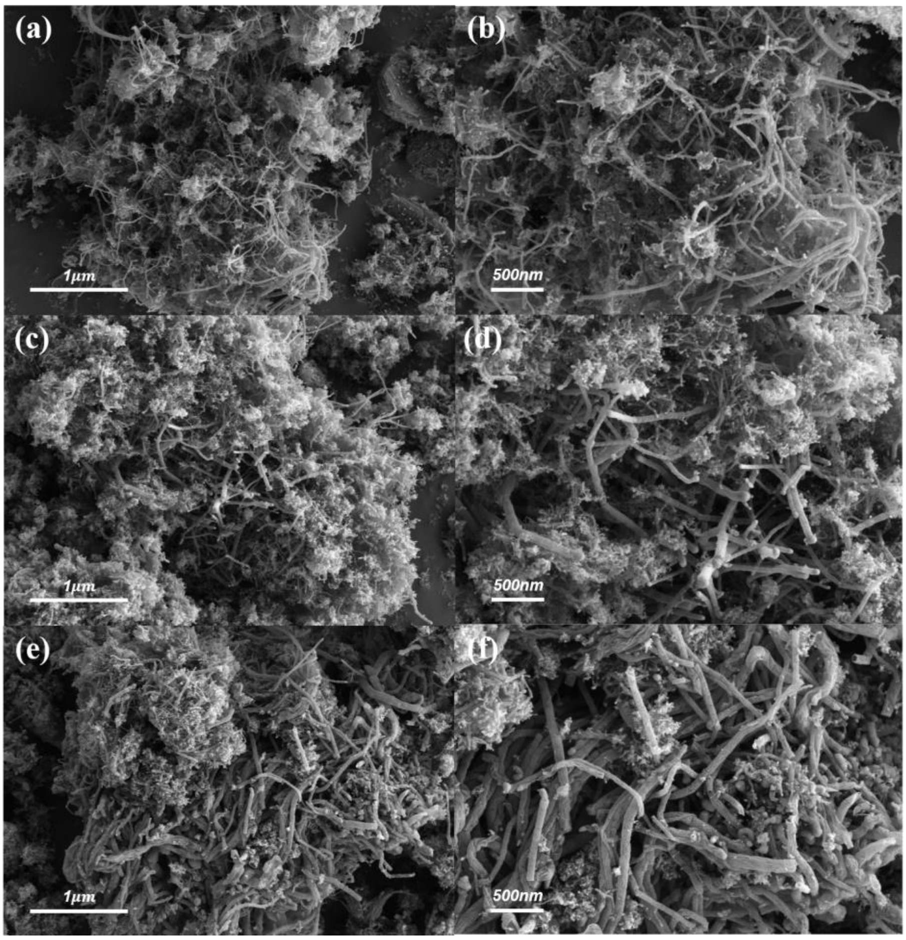


Fig. S2 SEM images of Co/NPCN$_{0.25}$, Co/NPCN$_{1.0}$ and Co/NPCN$_{1.5}$ catalysts

(a)(b) Co/NPCN$_{0.25}$; (c)(d) Co/NPCN$_{1.0}$; (e)(f) Co/NPCN$_{1.5}$

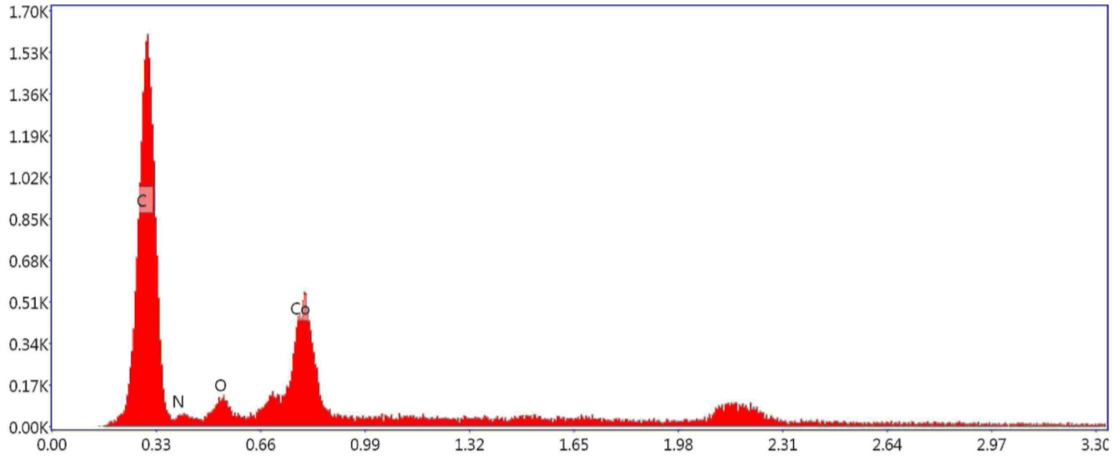


Fig. S3 EDS spectra of Co/$NPCN_{0.5}$

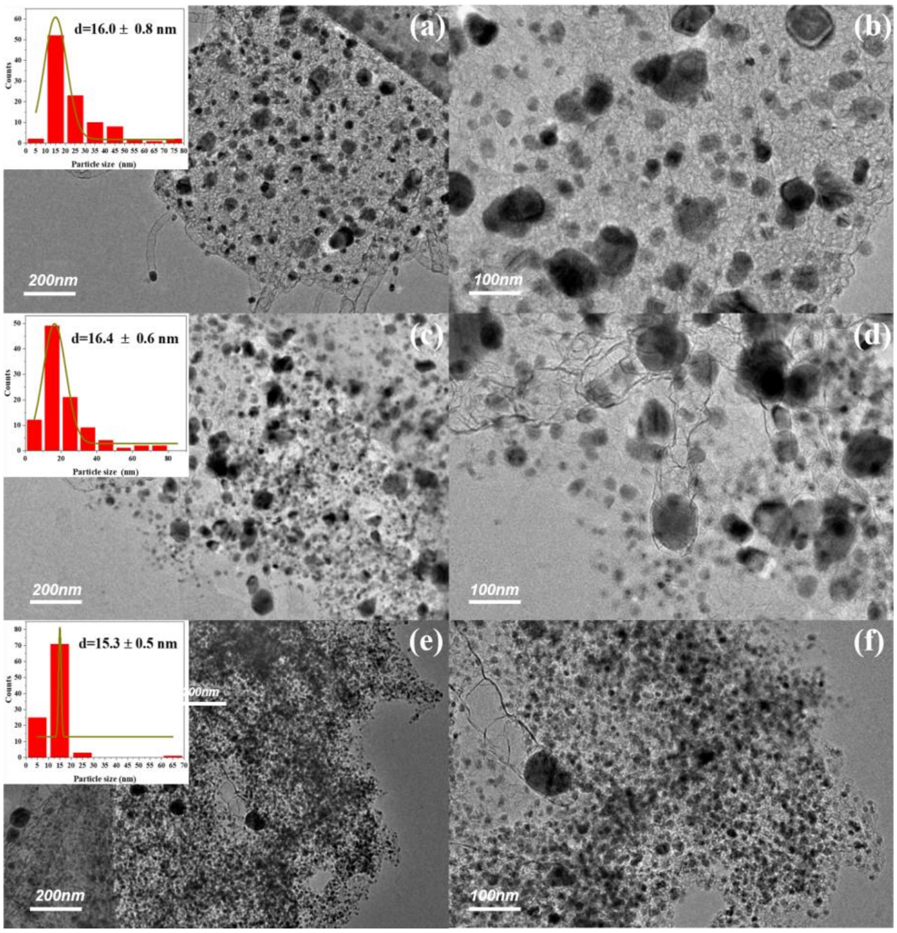


Fig. S4 TEM images of Co/NPCN catalysts with different g-C_3N_4 contents

(a), (b): Co/$NPCN_{0.25}$; (c), (d): Co/$NPCN_{1.0}$; (e), (f): Co/$NPCN_{1.5}$

Table S2 Determination of cobalt content in Co/NPCN with different g-C_3N_4 content by ICP-AES

Catalysts	Co wt. (%)
Co/$NPCN_{0.25}$	38.6
Co/$NPCN_{0.5}$	40.3
Co/$NPCN_{1.0}$	40.4
Co/$NPCN_{1.5}$	40.7

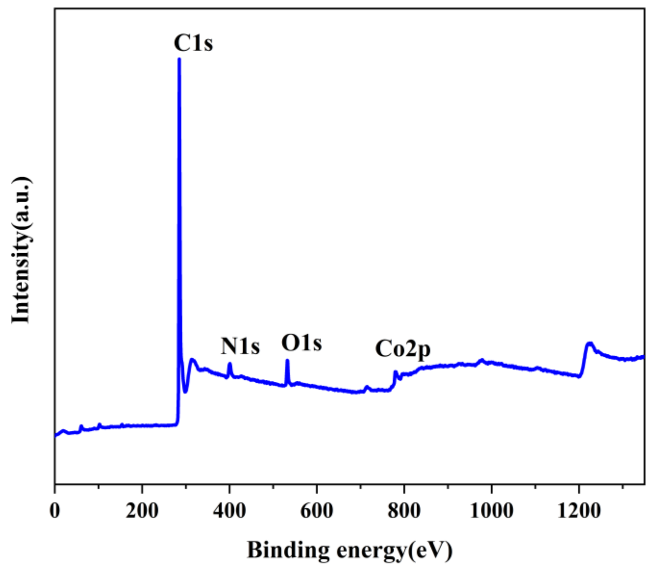
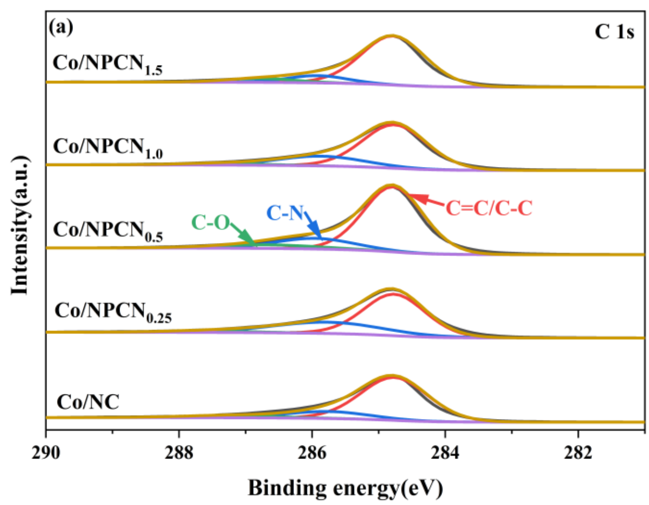


Fig. S5 XPS survey spectrum of Co/$NPCN_{0.5}$



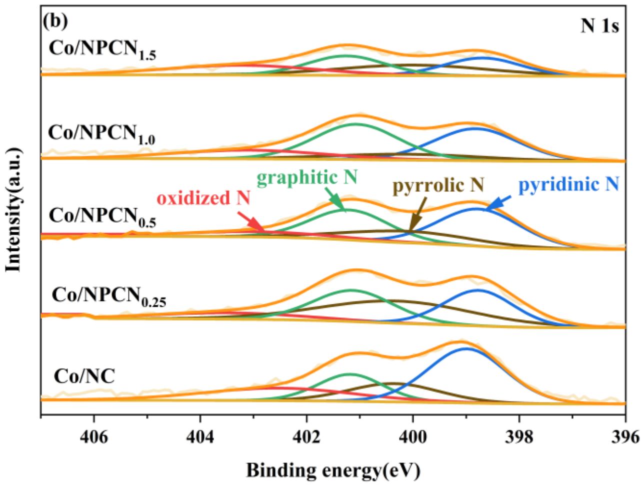


Fig. S6 XPS Spectra of Co/NPCN catalysts with different g-C_3N_4

(a) C 1s; (b) N 1s

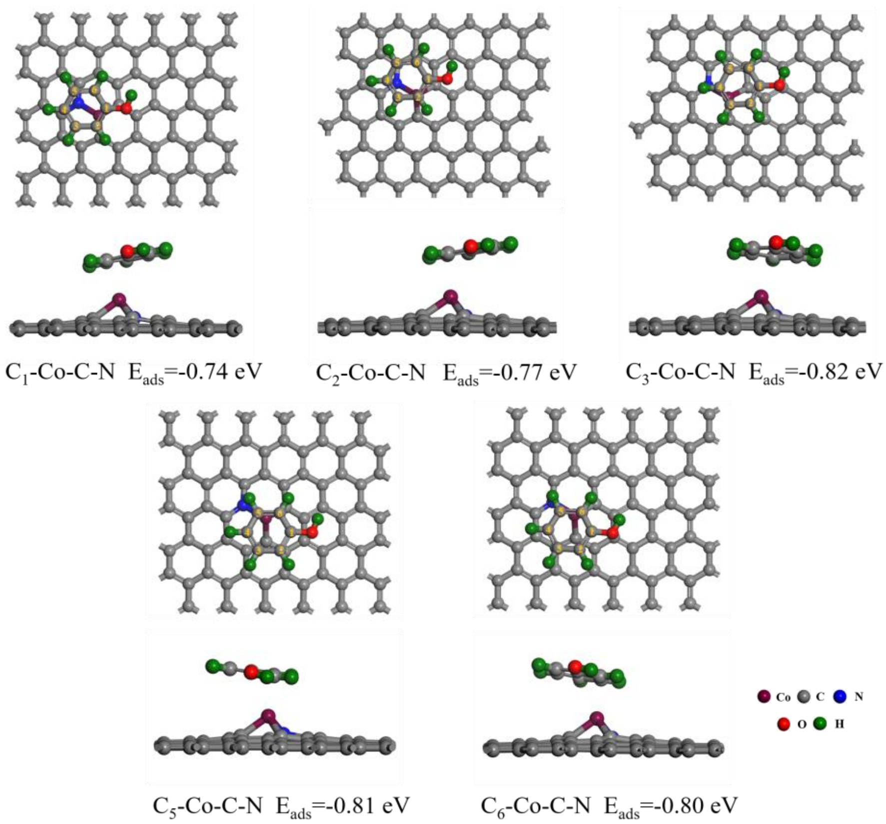


Fig. S7 Parallel stable adsorption configurations of C_1, C_2, C_3, C_5 and C_6 of phenol on Co sites of Co-C-N

The atomic colours of cobalt, carbon, nitrogen, oxygen and hydrogen are dark fuchsia, dark gray, blue, red and green, respectively.

Table S3 Adsorption energies of parallel and vertical adsorption of phenol and cyclohexanol on Co sites of Co-C-N

Adsorption atom	Adsorption energy (eV)				
	Parallel adsorption		Vertical adsorption		
C_3	phenol	-0.82	O	phenol	-0.79
	cyclohexanol	-0.36			
O	phenol	-0.79		cyclohexanol	-1.04
	cyclohexanol	-1.09			

Table S4 Catalytic performance of Co/NPCN catalysts at different pyrolysis temperatures

Catalysts	Phenol Conversion (%)	Cyclohexanol Selectivity (%)
Co/NPCN-600	0	--
Co/NPCN-700	72.8	100
Co/NPCN-800	97.8	100
Co/NPCN-900	29.6	100

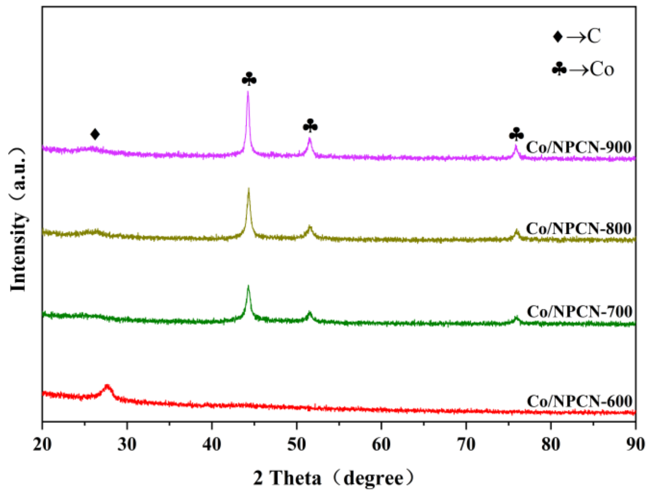


Fig. S8 XRD patterns of Co/NPCN catalysts at different pyrolysis temperatures

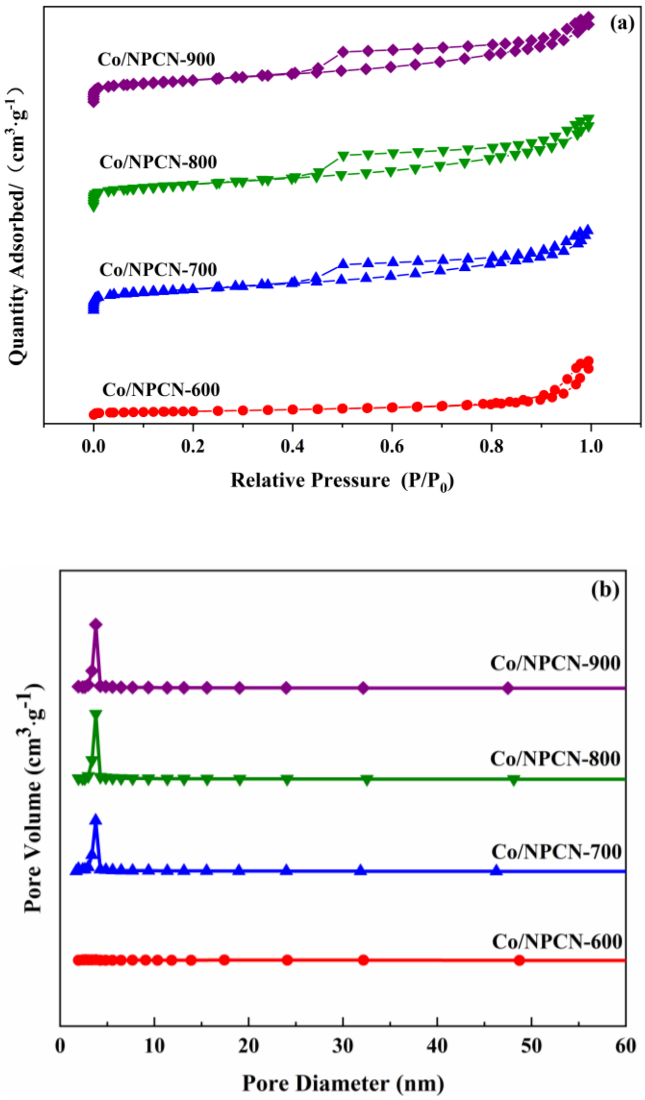


Fig. S9 N_2 adsorption-desorption isotherms (a) and pore size distribution curve (b)

Table S5 Structural parameters of Co/NPCN catalysts at different pyrolysis temperatures

Catalysts	S_{BET}（m^2/g）	V_t^b（cm^3/g）	D^c（nm）
Co/NPCN-600	79.1	0.3	18.1
Co/NPCN-700	320.1	0.5	6.1
Co/NPCN-800	342.6	0.8	8.7
Co/NPCN-900	330.3	0.5	6.3

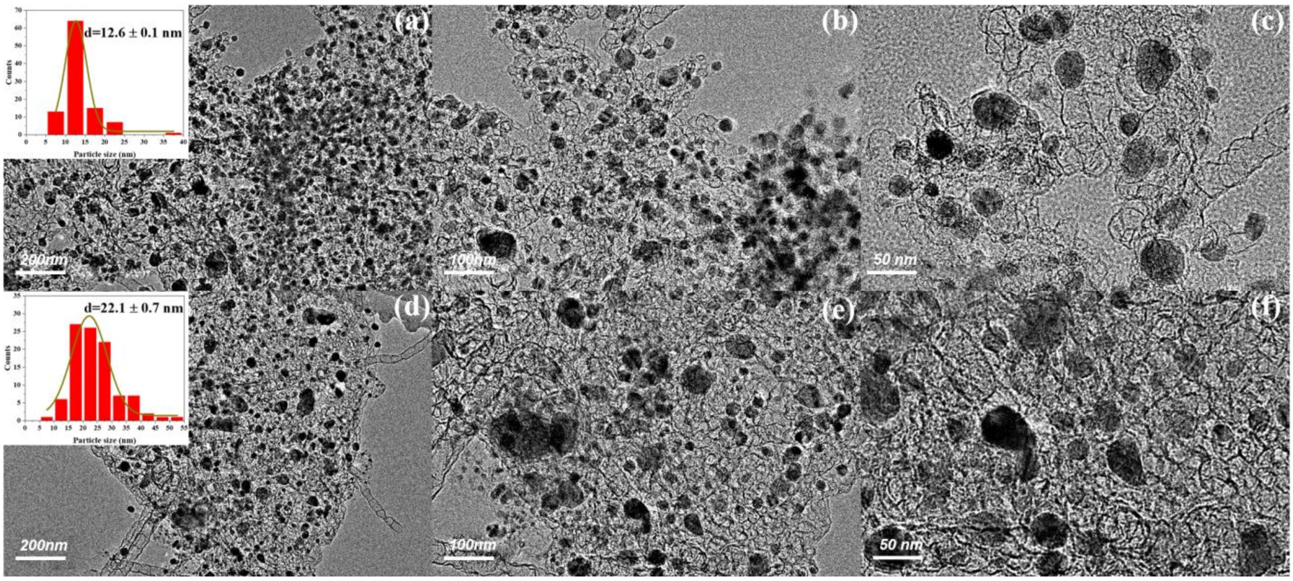


Fig. S10 TEM images of Co/NPCN catalysts at different pyrolysis temperatures

(a), (b), (c) Co/NPCN-700; (d), (e), (f) Co/NPCN-900

Table S6 Determination of cobalt content in Co/NPCN catalysts at different pyrolysis temperatures by ICP-AES

Catalysts	Co wt (%)
Co/NPCN-600	13.1
Co/NPCN-700	39.1
Co/NPCN-800	40.4
Co/NPCN-900	40.7

Table S7 Effects of different reaction pressures on selective hydrogenation of phenol

Pressure (MPa)	phenol Conversion (%)	cyclohexanol Selectivity (%)
1.0	96.4	100
1.5	96.9	100
2.0	97.8	100
2.5	97.8	100
3.0	97.9	100

Reaction conditions: catalyst 50mg, phenol 0.2mmol, H_2O 10mL, 120°C, 3h.

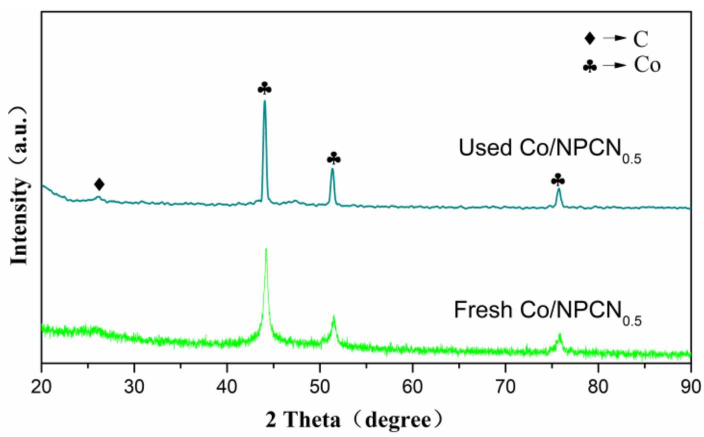


Fig. S11 XRD patterns of fresh and used Co/$NPCN_{0.5}$ catalyst