Highly selective oxidation of cyclohexene to 2-cyclohexene-1-one in water using molecular oxygen over Fe-Co-g-C$_3$N$_4$

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
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1. Experimental

Synthesis of different catalysts by conventional impregnation method: In a typical preparation, 0.4 g of pristine g-C$_3$N$_4$ mixed with 10 mL of deionized water was stirred and heated at 80°C in an oil bath. Next, 0.2 g of the metal precursors, FeCl$_3$ and Co(NO$_3$)$_2$·6H$_2$O, were added and the molar ratio of FeCl$_3$ to Co(NO$_3$)$_2$·6H$_2$O was 5. The mixed solution was continually heated at 100°C until removal of water. The resulting solid was then heated to 300°C at a rate of 3°C·min^{-1} and kept at this temperature for 3 h. Finally, the powder was obtained after cooling to room temperature. The obtained catalyst was denoted as Fe-Co/g-C$_3$N$_4$. Similarly, Fe/g-C$_3$N$_4$ or Co/g-C$_3$N$_4$ catalysts were prepared according to the same method as Fe-Co/g-C$_3$N$_4$ catalyst except that 0.2 g of FeCl$_3$ or Co(NO$_3$)$_2$·6H$_2$O was added separately.
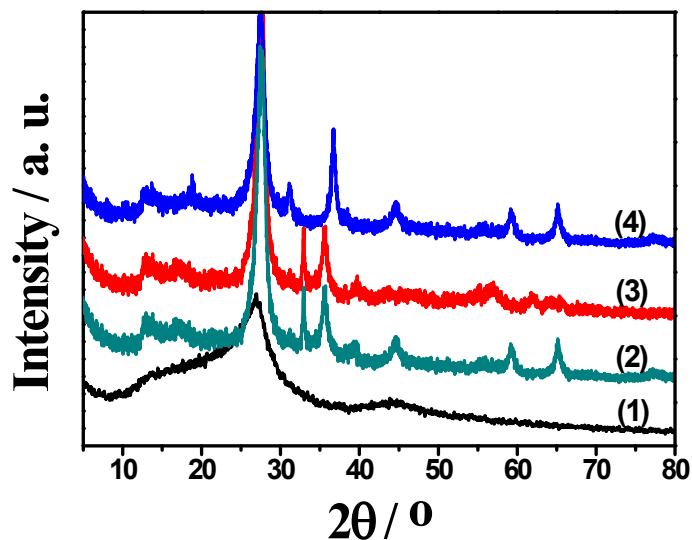
2. Results

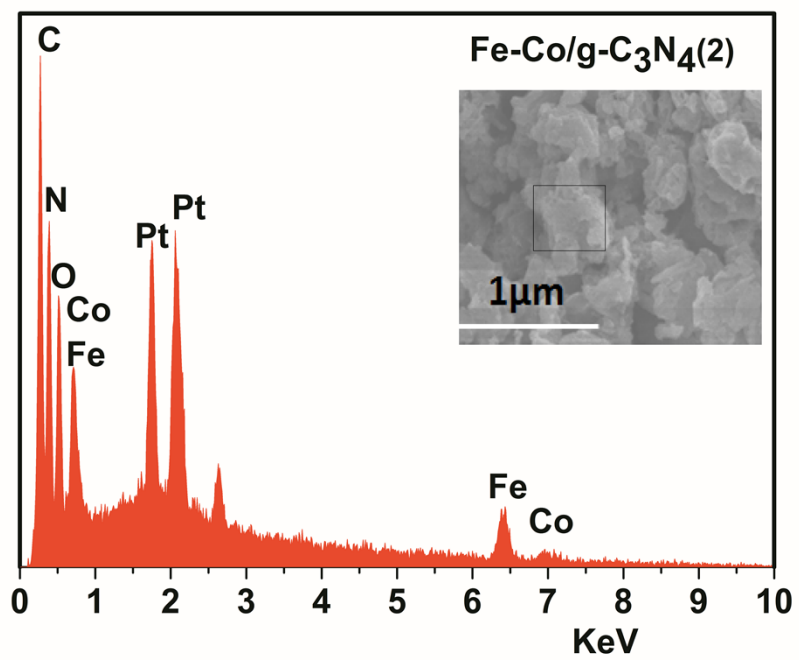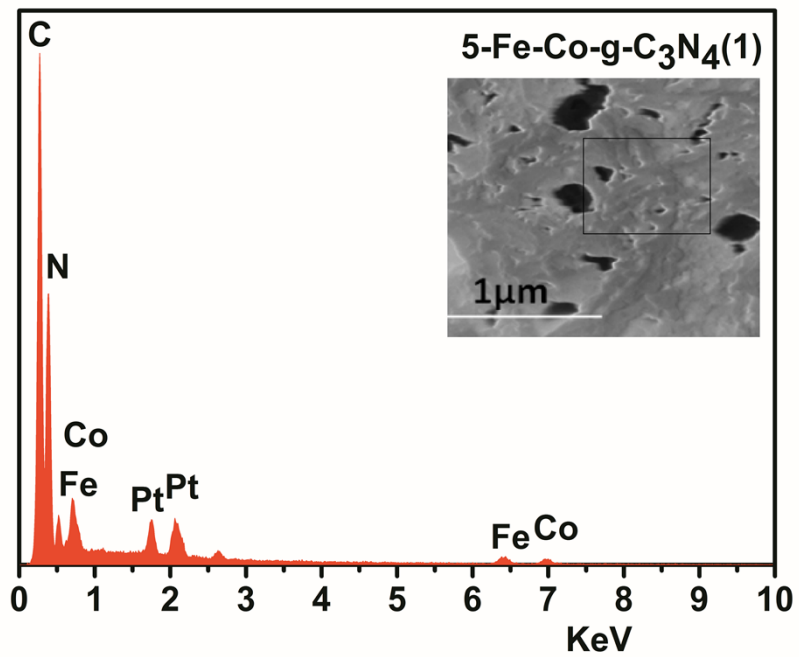Table S1. Catalytic activity of g-C$_3$N$_4$ doped with various metals for the oxidation of cyclohexene[a]

Entry	Catalysts	Conversion (%)	Selectivity (%)			
			![O ketone]	![OH alcohol]	![diol]	Others
1	Fe/g-C$_3$N$_4$	7.2	72.5	9.4	14.2	3.9
2	Co/g-C$_3$N$_4$	33.74	66.1	26.1	6.1	1.7
3	Fe-Co/g-C$_3$N$_4$	13.8	68.0	22.0	9.3	0.7
4	Fe-Co-g-C$_3$N$_4$	21.8	95.5	1.2	1.9	1.4

**Figure S1.** XRD patterns of 5-Fe-Co-g-C_3N_4 (1), Fe-Co/g-C_3N_4 (2), Fe/g-C_3N_4 (3), Co/g-C_3N_4 (4). It is can be seen that XRD pattern of 5-Fe-Co-g-C_3N_4 is obviously different from that of Fe-Co/g-C_3N_4, Fe/g-C_3N_4 or Co/g-C_3N_4. There were no peaks originating from Fe or Co species in 5-Fe-Co-g-C_3N_4 sample, due to the formation of Fe-N or Co-N bonds through the chemical coordination of Fe or Co species with g-C_3N_4. However, the diffraction peak for Fe or Co was clearly observed in Fe-Co/g-C_3N_4, Fe/g-C_3N_4 or Co/g-C_3N_4 sample, and Fe or Co species mainly existed in the form of Fe_3O_4 and Co_3O_4.

5-Fe-Co-g-C$_3$N$_4$(1)

1μm

C

N

Co

Fe

Pt Pt

Fe Co

KeV

Fe-Co/g-C$_3$N$_4$(2)

1μm

C

N

O

Co

Fe

Pt Pt

Fe

Co

KeV
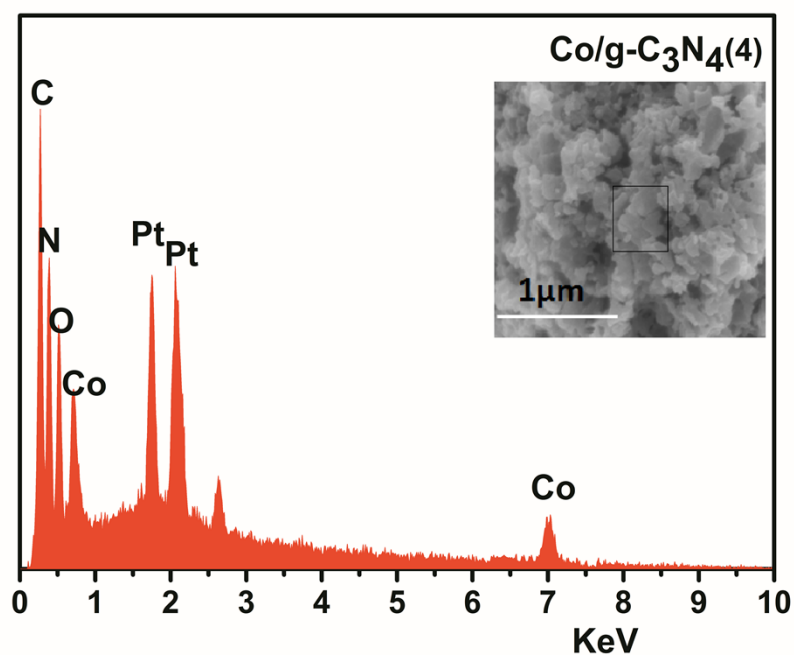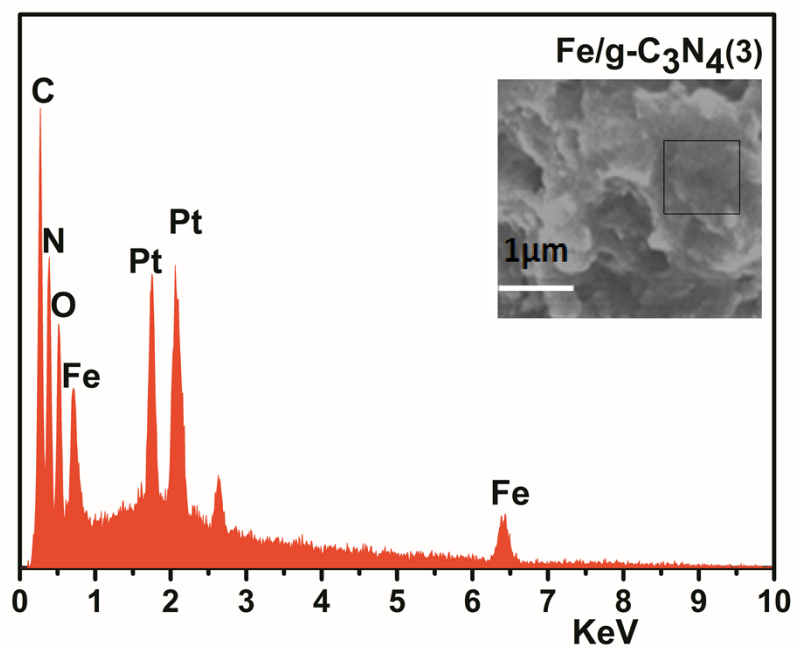
Figure S2. Energy dispersive X-ray (EDX) spectra and SEM images (Inset) of 5-Fe-Co-g-C_3N_4 (1), Fe-Co/g-C_3N_4 (2), Fe/g-C_3N_4 (3), Co/g-C_3N_4 (4). It shows the presence of C, N, O, Fe and Co in Fe-Co/g-C_3N_4, Fe/g-C_3N_4 or Co/g-C_3N_4 samples. However, only the small amount of O was found in 5-Fe-Co-g-C_3N_4 sample. Pt

element comes from sample spraying for better conductivity so that the better SEM images can be obtained.
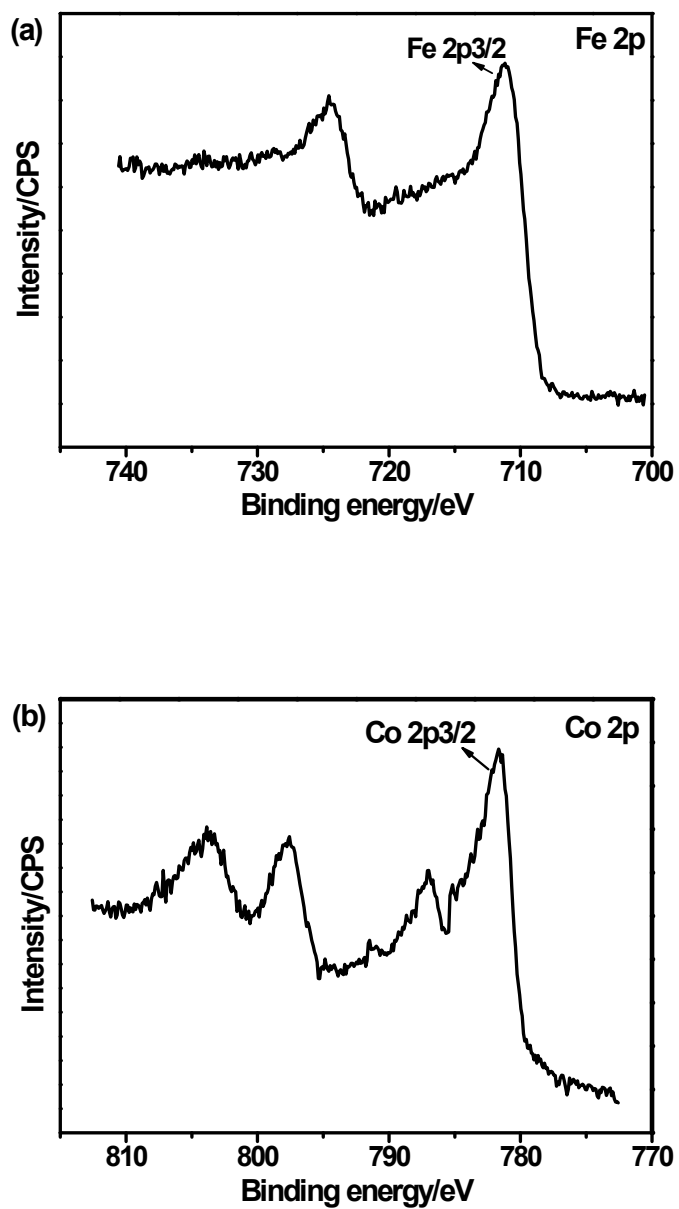
Figure S3. XPS spectra of Fe2p (a), and Co2p (b) in the Fe-Co/g-C_3N_4.