

Supplementary information of  
Covalent triazine framework supported non-noble metal  
nanoparticles with superior activity for catalytic hydrolysis of  
ammonia borane: from mechanistic study to catalyst design

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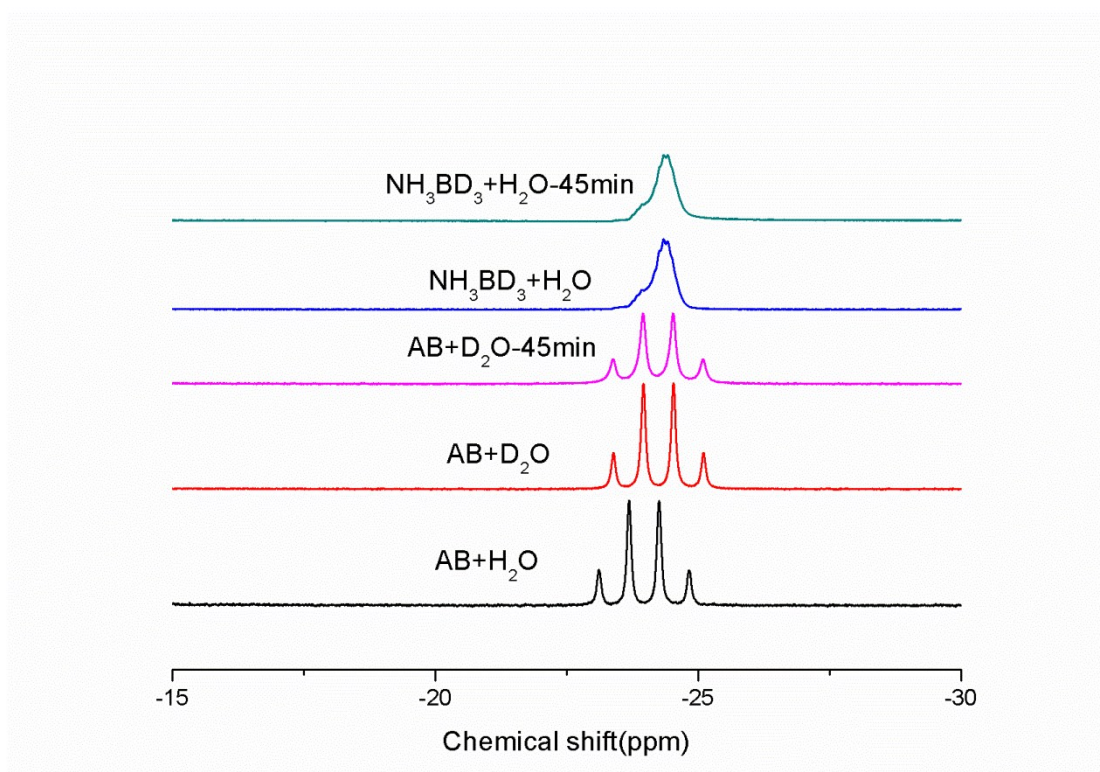
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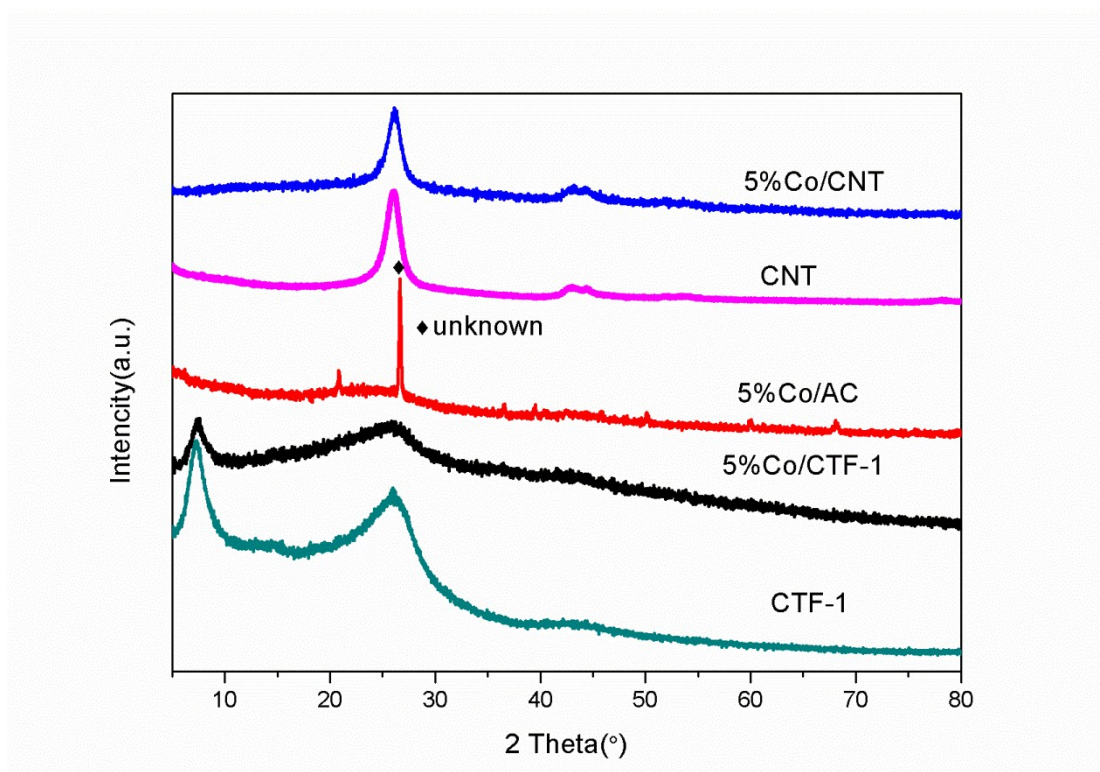
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**Figure S1.**  $^{11}\text{B}$  NMR spectra of the AB and  $\text{NH}_3\text{BD}_3$  dissolving in  $\text{D}_2\text{O}$  and  $\text{H}_2\text{O}$  measured at different time.



**Figure S2.** XRD patterns of CTF-1, CNT, 5%Co/CTF-1, 5%Co/CNT, 5%Co/AC.

**Table S1. The surface areas before and after loading ( $S_{BET}$ ), Co contents determined by ICP, and average particle sizes of CTF-1, CNT and AC supported catalysts.**

<b>Catalysts and supports</b>	<b>Co contents (wt%)</b>	<b>Average particle size(nm)</b>	<b><math>S_{BET}</math> Before loading(m<sup>2</sup>/g)</b>	<b><math>S_{BET}</math> After loading(m<sup>2</sup>/g)</b>
<b>5%Co/CTF-1</b>	<b>4.48</b>	<b>3.3</b>	<b>947</b>	<b>726</b>
<b>5%Co/CNT</b>	<b>4.24</b>	<b>7.3</b>	<b>160</b>	<b>156</b>
<b>5%Co/AC</b>	<b>4.34</b>	<b>-</b>	<b>714</b>	<b>685</b>
<b>3%Co/CTF-1</b>	<b>2.83</b>	<b>-</b>	<b>-</b>	<b>-</b>

**Table S2. Selective activities in terms of TOF values ( $\text{mol H}_2 \cdot (\text{mol catalyst})^{-1} \cdot \text{min}^{-1}$ ) and activation energy  $E_a$  (kJ/mol) of the non-noble metal catalysts tested in hydrogen generation from the hydrolysis of AB so far.**

Catalyst	$n_{\text{metal}}/n_{\text{AB}}$	TOF	$E_a$ (kJ/mol)	Reference
10wt% Co/ $\gamma$ -Al <sub>2</sub> O <sub>3</sub>	0.018	2.30	62	1
10 wt %Co/SiO <sub>2</sub>	0.018	2.3	-	1
10 wt % Co/C	0.018	2.92	-	1
Co/zeolite	0.02	5.36	56	2
PVP-Co	0.025	4.80	46	3
PSMA-Co	0.001	25.7	34.22	4
Co/graphene	0.05	13.8	32.75	5
G6-OH(Co <sub>60</sub> )	0.013	10	50.2	6
Ni/C	0.0425	8.8	28	7
5%Co/CTF-1	0.05	33.5	42.7	This study
3%Co/CTF-1	0.03	42.3	-	This study
5%Co/CNT	0.05	8.5	46.9	This study
5%Co/AC	0.05	5.8	47.2	This study
5%Ni/CTF-1	0.05	8.75	-	This study
5%Ni/CNT	0.05	5.4	-	This study
5%Ni/AC	0.05	2.6	-	This study
Au@Co	0.02	13.7	-	8
Co <sub>35</sub> Pd <sub>65</sub>	0.024	22.7	27.5	9
Ag@CoNi/graphene	0.05	15.89	36.15	10
PEI-GO/Co	0.11	39.9	28.2	11
Ni <sub>2</sub> P	0.054	40.4	44.6	12
Ni@MCS-30	0.016	30.7	-	13
Pt black	0.018	14	-	14
2 wt.% Pd/ $\gamma$ -Al <sub>2</sub> O <sub>3</sub>	0.018	1.3	-	14

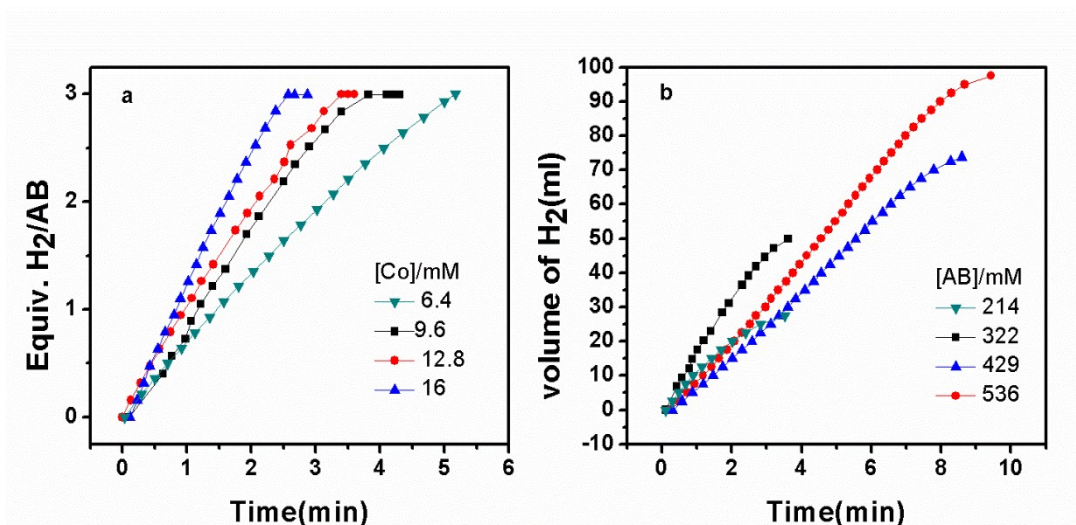


Figure S3. The Plots of volume of H<sub>2</sub> vs. time from AB hydrolysis catalyzed by the Co/CTF-1 catalyst at different catalyst (a) and AB concentrations (b) at T =298 K.

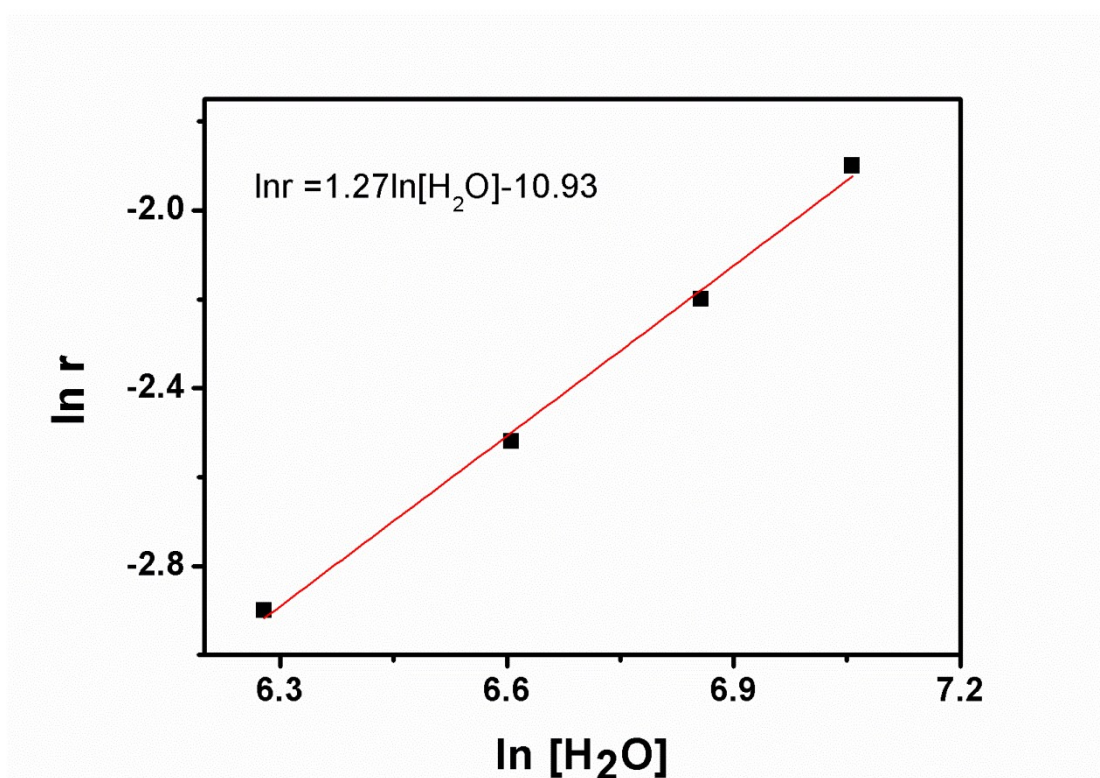


Figure S4. The plot of hydrogen generation rate versus the concentration of H<sub>2</sub>O in natural logarithmic scale,  $\ln(\text{rate}) = 1.27 \ln [H_2O] - 10.93$

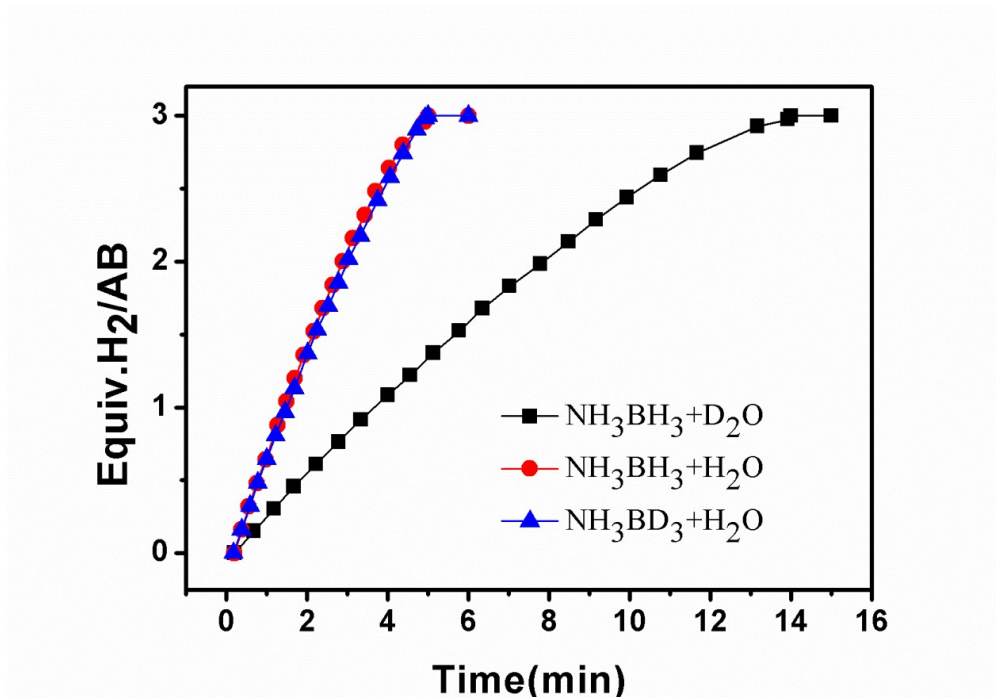


Figure S5. Kinetic isotope effect of hydrolytic AB catalyzed by 5%Co/CTF-1 at room temperature with  $n_{\text{Co}}:n_{\text{AB}}=0.05:1$  for  $\text{NH}_3\text{BH}_3$  in  $\text{D}_2\text{O}$  (black),  $\text{NH}_3\text{BD}_3$  in  $\text{H}_2\text{O}$  (blue) and  $\text{NH}_3\text{BH}_3$  in  $\text{H}_2\text{O}$  (red).

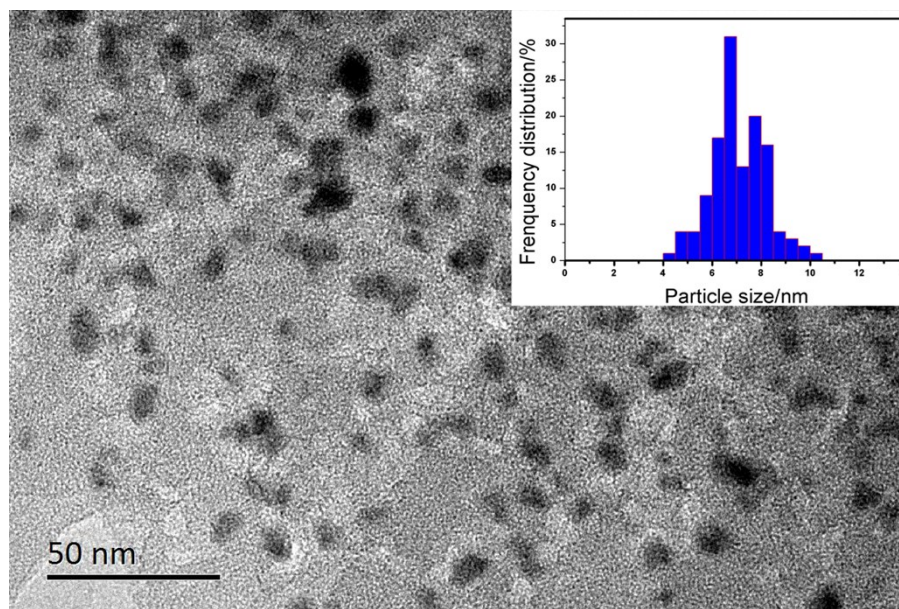
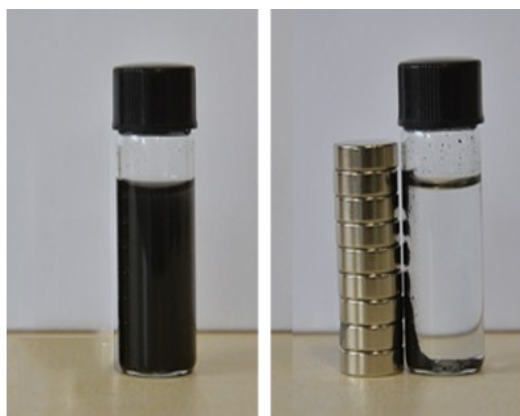
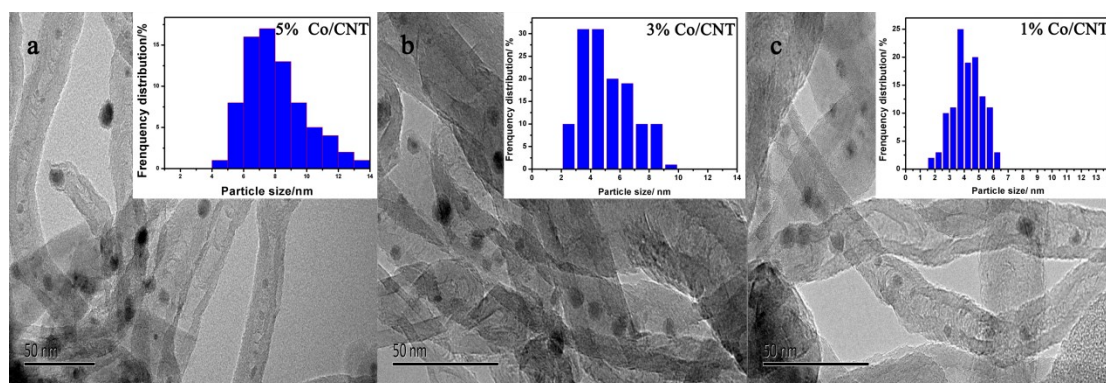


Figure S6. TEM image and corresponding size histograms of Co/CTF-1 NPs after 5 recycle times.



**Figure S7. Left. After hydrolysis reaction; Right. Separation of catalyst by magnet.**



**Figure S8. TEM images and corresponding size histograms of a. 5%Co/CNT, b. 3%Co/CNT, c. 1%Co/CNT. The average size is calculated from at least 100 NPs.**

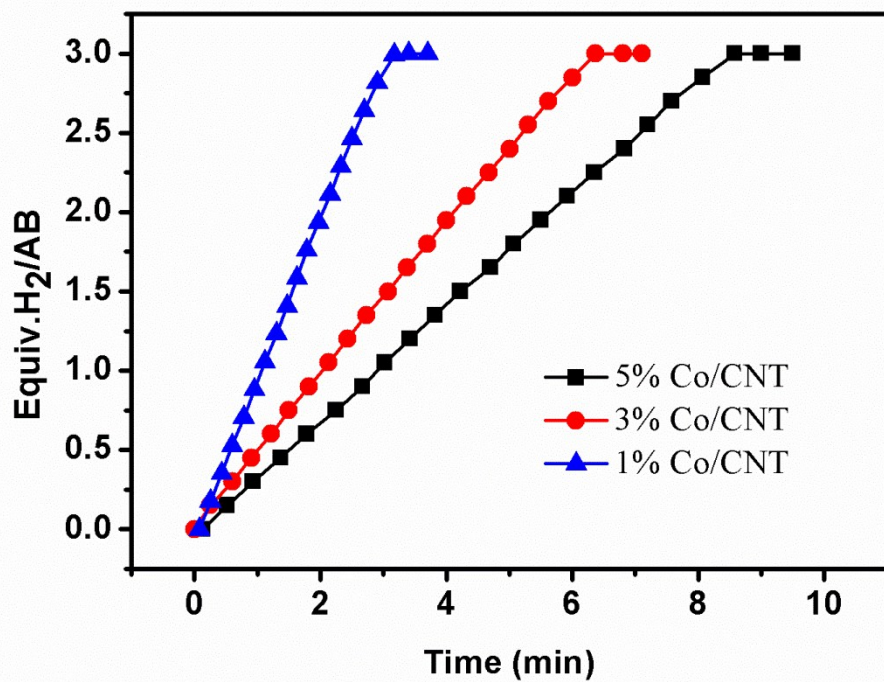
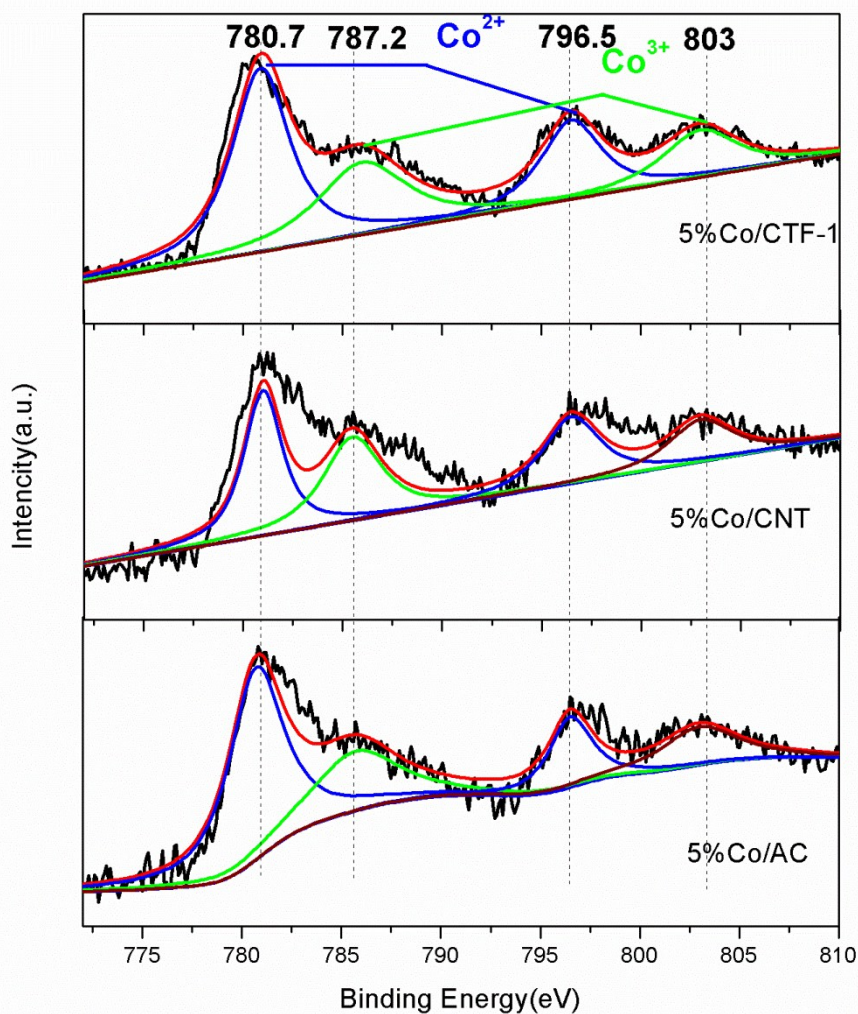


Figure S9. Plot of time vs volume of H<sub>2</sub> generated from AB hydrolysis catalyzed by 5%Co/CNT, 3%Co/CNT, 1%Co/CNT. ( [AB] = 322 mM, 5ml,  $n_{\text{metal}}/n_{\text{AB}}=0.05$ )





**Figure S10. XPS spectra of 5%Co/CTF, 5%Co/CNT, 5%Co/AC before Ar sputtering.**

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