Supporting Information

Base-promoted hydrolytic dehydrogenation of ammonia borane catalyzed by noble-metal-free nanoparticles

Qilu Yao,[#] Kun Yang,[#] Xiaoling Hong, Xiangshu Chen* and Zhang-Hui Lu*

Institute of Advanced Materials (IAM), College of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang, 330022, P. R. China.

[#]*These authors contributed equally to this work.*

**Email: cxs66cn@jxnu.edu.cn; luzh@jxnu.edu.cn*

Table S1 The pH values of the solution at different steps of the preparation of the $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs and the hydrolysis of AB catalyzed by this catalyst.

Step	Condition	pH
1	Before reduction of metals	5.3
2	After reduction by $NaBH_4$ (20 mg)	10.0
3	After addition of NaOH (1 M)	13.65
4	After addition of NH_3BH_3 (1 mmol)	13.65
5	After release of 3.0 equivalent of gases	13.52

Table S2 The pH values of the reaction solution by add different additives before the hydrolysis of AB.

Additive	**pH**
Without addition additive	10.2
After addition NaOH	13.65
After addition KOH	13.65
After addition Na_2CO_3	11.0
After addition NH_4Cl	8.1
After addition CH_3COONH_4	8.4
After addition $NH_3 \cdot H_2O$ (2 mL)	11.3

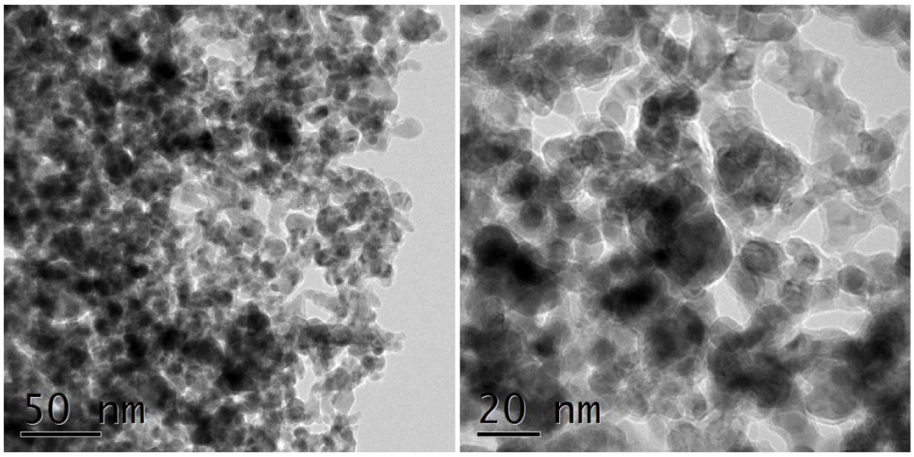

Fig. S1 TEM images of CuCo NPs.

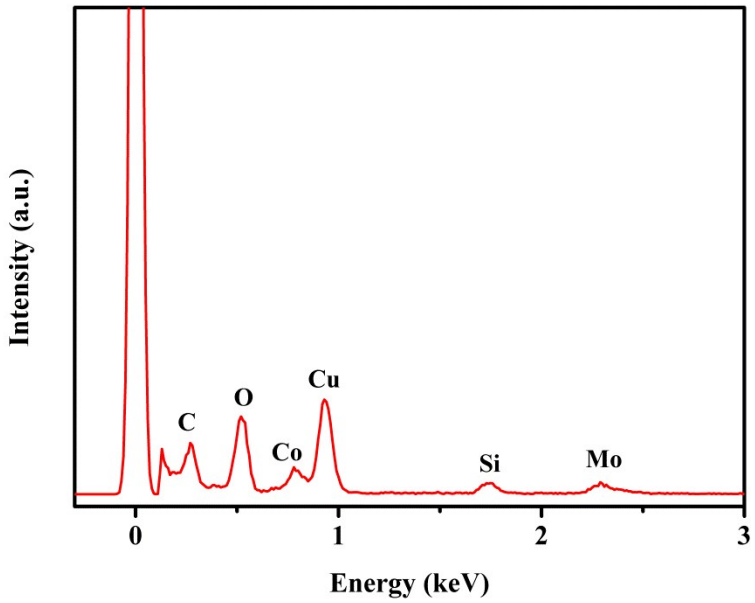

Fig. S2 EDX spectrum of $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs.

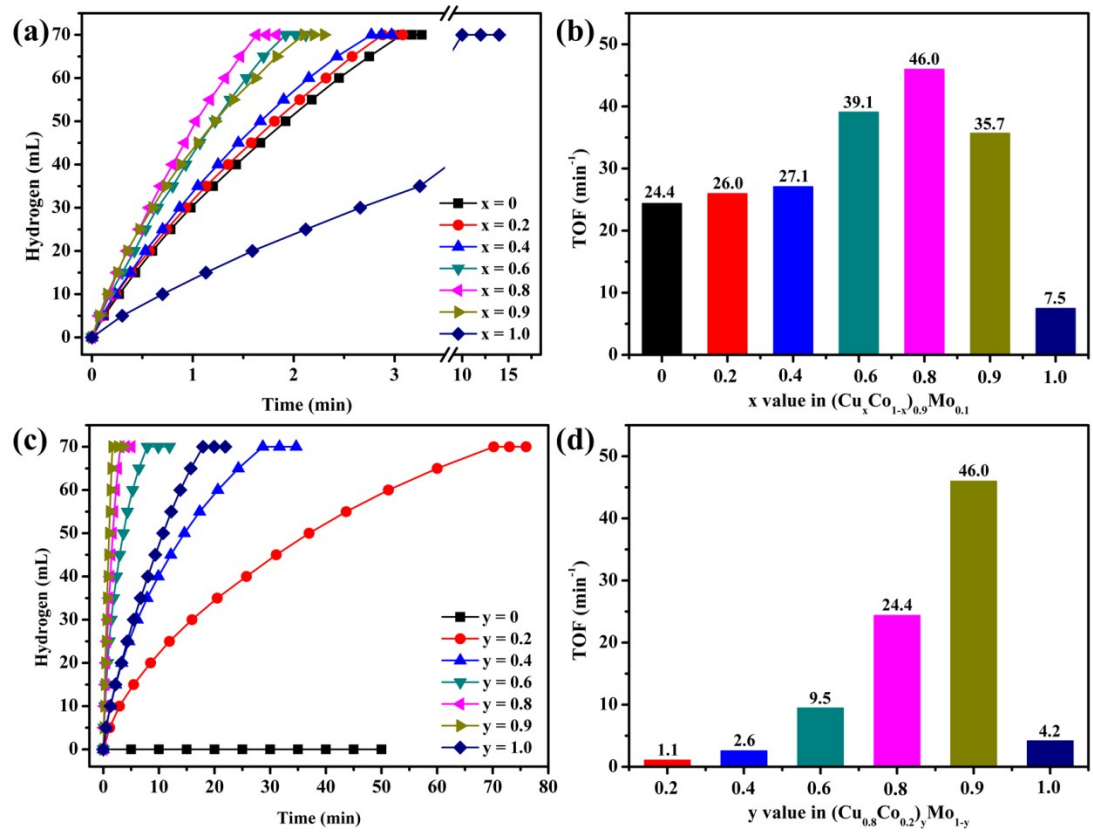

Fig. S3 Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) catalyzed by (a) $(Cu_xCo_{1-x})_{0.9}Mo_{0.1}$ NPs and (c) $(Cu_{0.8}Co_{0.2})_yMo_{1-y}$ NPs at 298 K; (b,d) the corresponding TOF values (n_{metal} = 0.04 mmol).

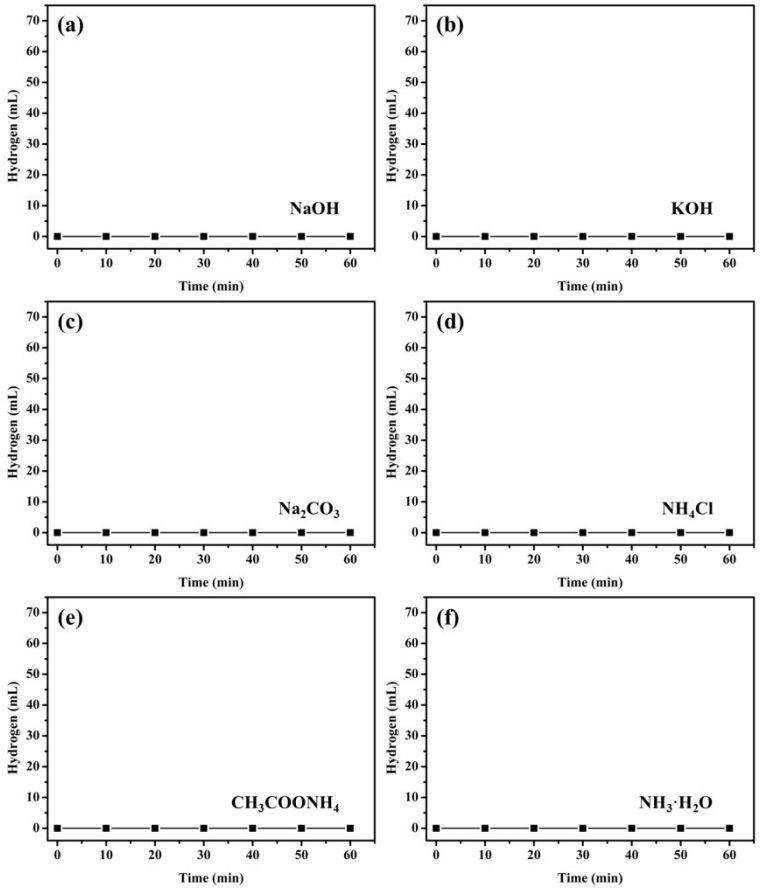

Fig. S4 Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) in the presence of 1 M (a) NaOH, (b) KOH, (c) Na_2CO_3, (d) NH_4Cl, (e) CH_3COONH_4, and (f) $NH_3 \cdot H_2O$ (2 mL) at 298 K.

No hydrogen generation is observed for NaOH, KOH, Na_2CO_3, NH_4Cl, CH_3COONH_4, and $NH_3 \cdot H_2O$ toward the hydrolysis of AB in the absence of $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs (Fig. S4), suggesting that these additives have no catalytic activity for the hydrolysis of AB.

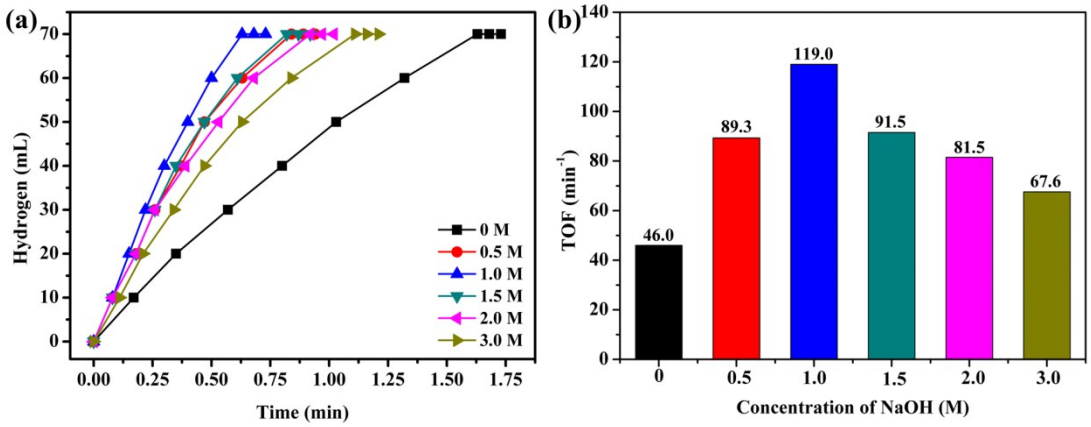

Fig. S5 (a) Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) with different molar ratios of NaOH catalyzed by $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs at 298 K and (b) the corresponding TOF values (n_{metal} = 0.04 mmol).

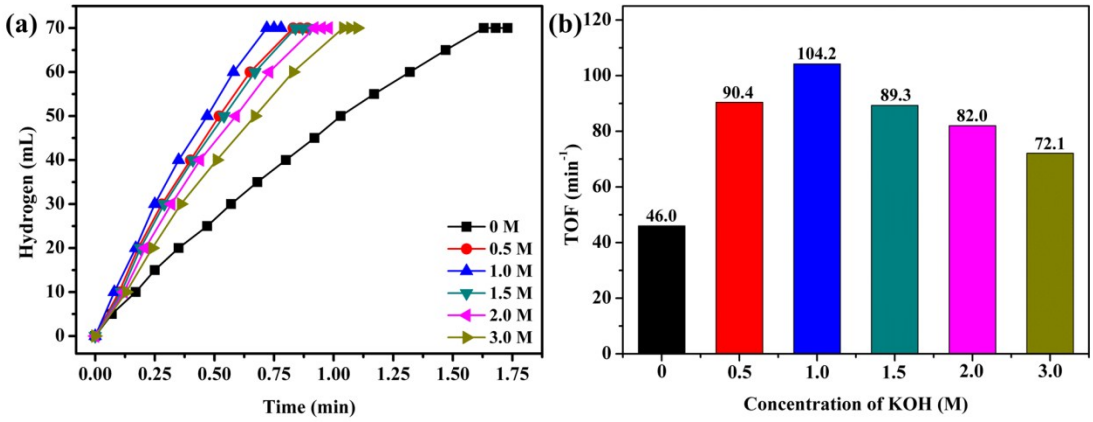

Fig. S6 (a) Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) with different molar ratios of KOH catalyzed by $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs at 298 K and (b) the corresponding TOF values (n_{metal} = 0.04 mmol).

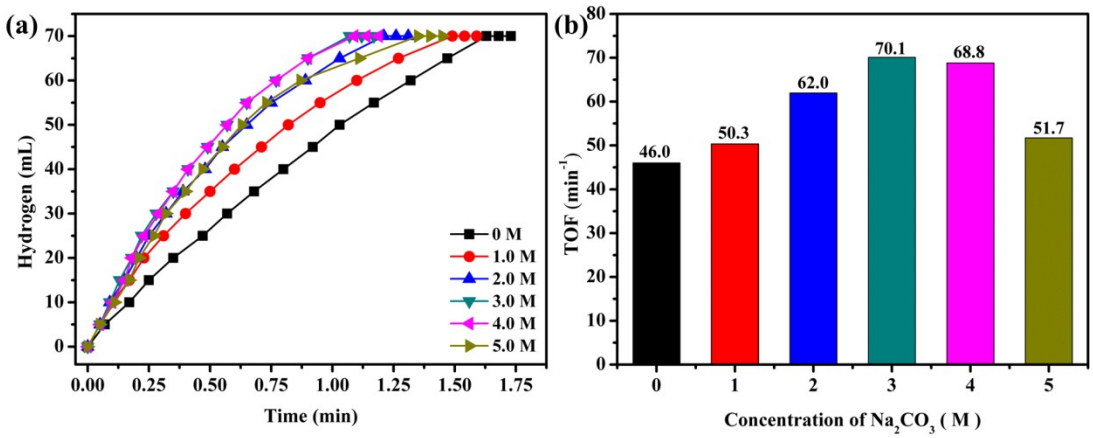

Fig. S7 (a) Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) with different molar ratios of Na_2CO_3 catalyzed by $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs at 298 K and (b) the corresponding TOF values (n_{metal} = 0.04 mmol).

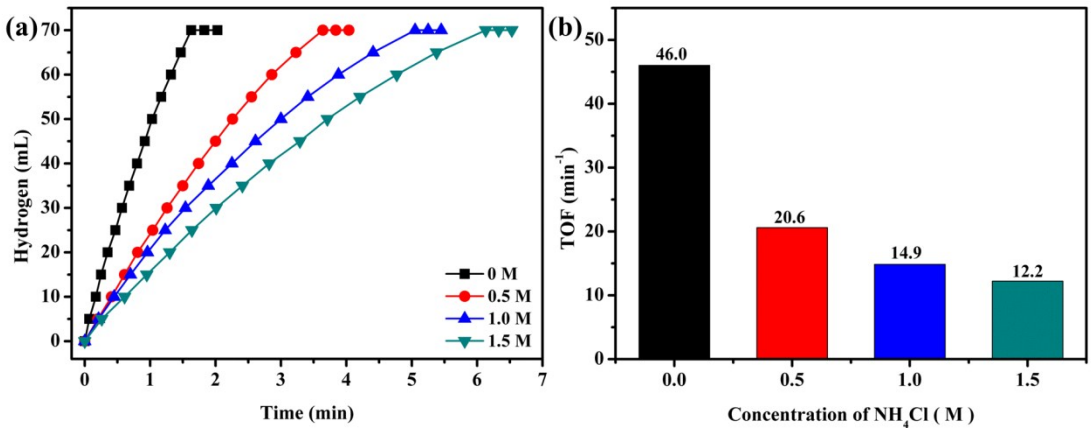

Fig. S8 (a) Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) with different molar ratios of NH_4Cl catalyzed by $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs at 298 K and (b) the corresponding TOF values (n_{metal} = 0.04 mmol).

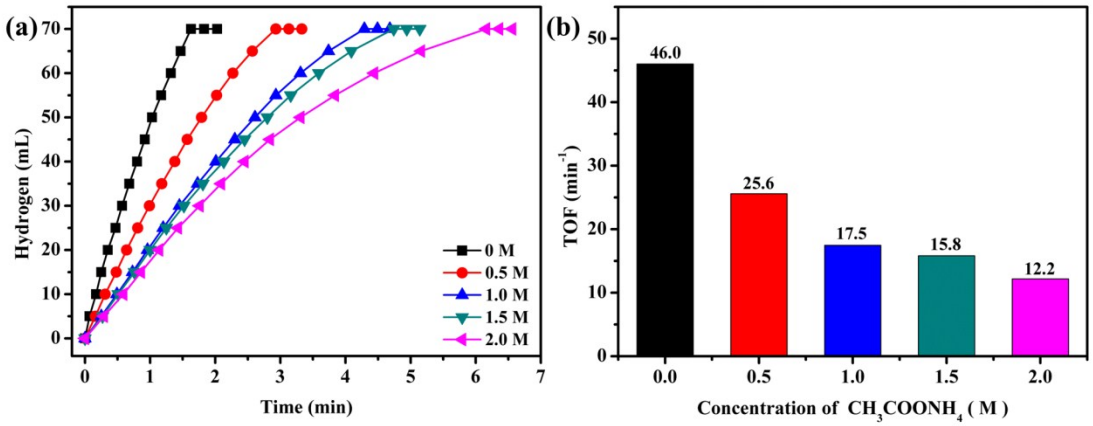

Fig. S9 (a) Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) with different molar ratios of CH_3COONH_4 catalyzed by $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs at 298 K and (b) the corresponding TOF values (n_{metal} = 0.04 mmol).

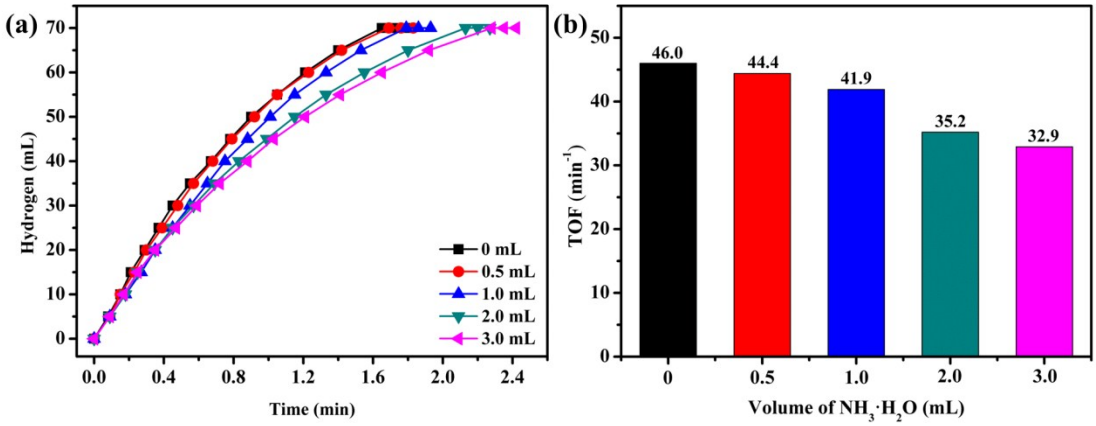

Fig. S10 (a) Hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) with different volumes of $NH_3 \cdot H_2O$ catalyzed by $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs at 298 K and (b) the corresponding TOF values (n_{metal} = 0.04 mmol).

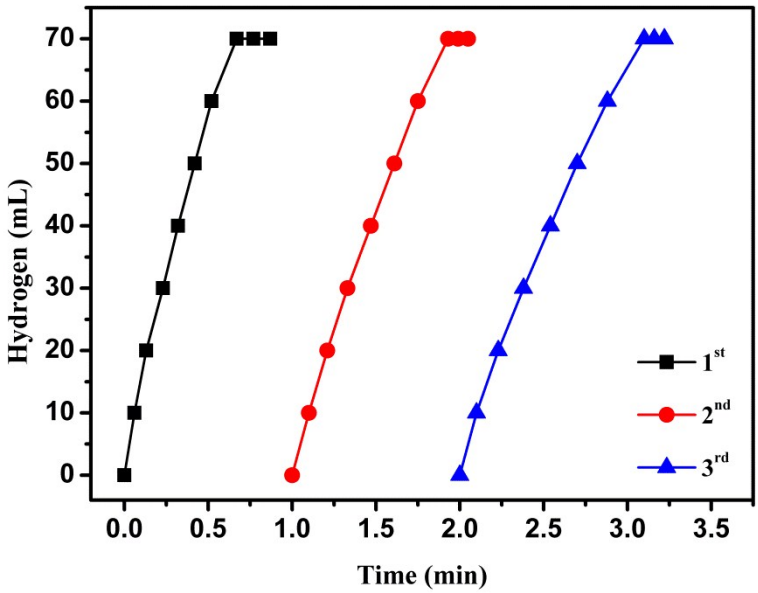

Fig. S11 Stability test for hydrogen generation from the hydrolysis of AB (0.20 M, 5 mL) catalyzed by $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs at 298 K (n_{metal} = 0.04 mmol).

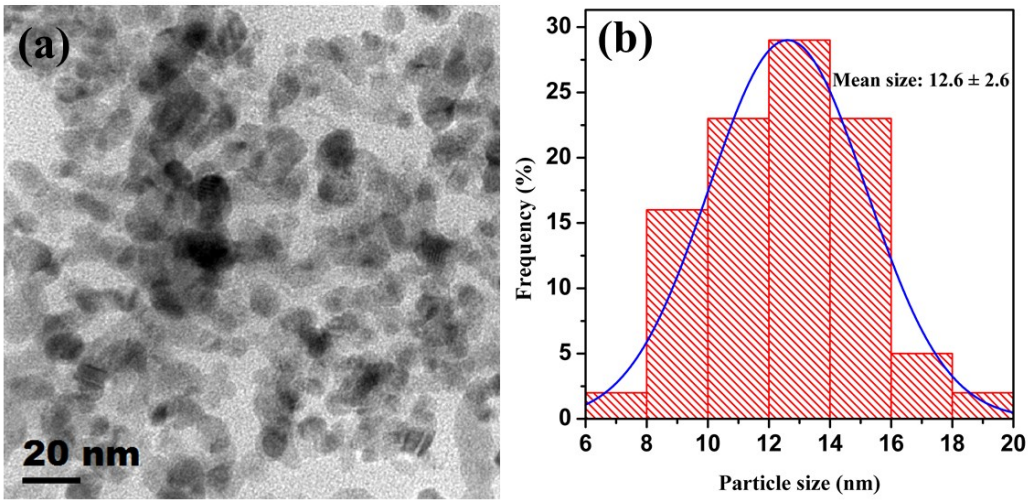

Fig. S12 (a) TEM image and (b) size distribution of $Cu_{0.72}Co_{0.18}Mo_{0.1}$ NPs after the stability test.

The turnover frequency (*TOF*) reported in this work is an apparent *TOF* value based on the number of metal atoms in catalyst, which is calculated from the equation as follow:

$$TOF = \frac{n_{H_2}}{n_{metal} \times t} \qquad \text{(S1)}$$

Where n_{H_2} is the mole number of generated H_2, n_{metal} is the mole number of Cu+Co+Mo in catalyst and t is the completed reaction time in minute.