

Support Information

Highly dehydrogenation of ammonia borane by core-shell heterostructure catalysts with carbon template-assisted synthesis

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Physicochemical Characterization

The X-ray powder diffraction (XRD) patterns of the samples were recorded by a German Brock D8 ADVANCE X-ray diffractometer. The morphologies of the samples were characterized by FEI Quanta 650 scanning electron microscope (SEM). Transmission electron microscopy (TEM) and high resolution TEM (HRTEM) images were obtained by US FEI Tecnai G2 F20 transmission electron microscopy. X-ray photoelectron spectroscopy (XPS) was analyzed by Thermo Scientific K-Alpha X-ray photoelectron spectrometer. The metal concentration in catalyst was determined by inductively coupled plasma emission spectrometry.

Catalytic experiment and stability test

A mixture of 25 mg catalyst and 23mL deionized water was placed in a glass container and magnetically stirred to disperse the mixture evenly in the ultra-pure water. One end of the flask is connected to a measuring tube to measure the volume of gas, and the other end is sealed with a rubber plug. The flask is placed in a water bath at 30°C. Ammonia borane (2 mL, 0.375 mol·L⁻¹) was injected into the reaction flask through a syringe under magnetic stirring, and the hydrolyzed hydrogen reaction of ammonia borane began. Observe the water level of the gas pipe every 30s to record the volume of hydrogen released. The reaction is complete when no more gas is observed escaping.

To calculate the activation energy of the reaction, Co₁Cu₁/Cu_{0.76}Co_{2.24}O₄ catalyzed the hydrolysis of AB at different temperatures (298, 303, 308 and 313 K). At the completion of the previous cycle, without separating and washing the used catalyst, 2 mL of AB was quickly injected into the container and the amount of hydrogen produced for each cycle was recorded.

The apparent activation energy (E_a) was calculated with eq. (1)

$$\ln rate = - \left(\frac{E_a}{RT} \right) + C \quad (1)$$

Where T was the reaction temperature (K), R was the molar gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), and C was the corresponding constant.

The TOF value was determined on the basis of the reported literature using the eq. (2)

$$TOF = \frac{n_{H_2}}{t \times n_{Co}} \quad (2)$$

Where n_{H_2} was the amount of hydrogen generated (mol), t was the corresponding reaction time (min), and n_{Co} was determined based on the amount of Co in the feeding catalysts calculated from the catalyst dosage and the mass fraction (mol).

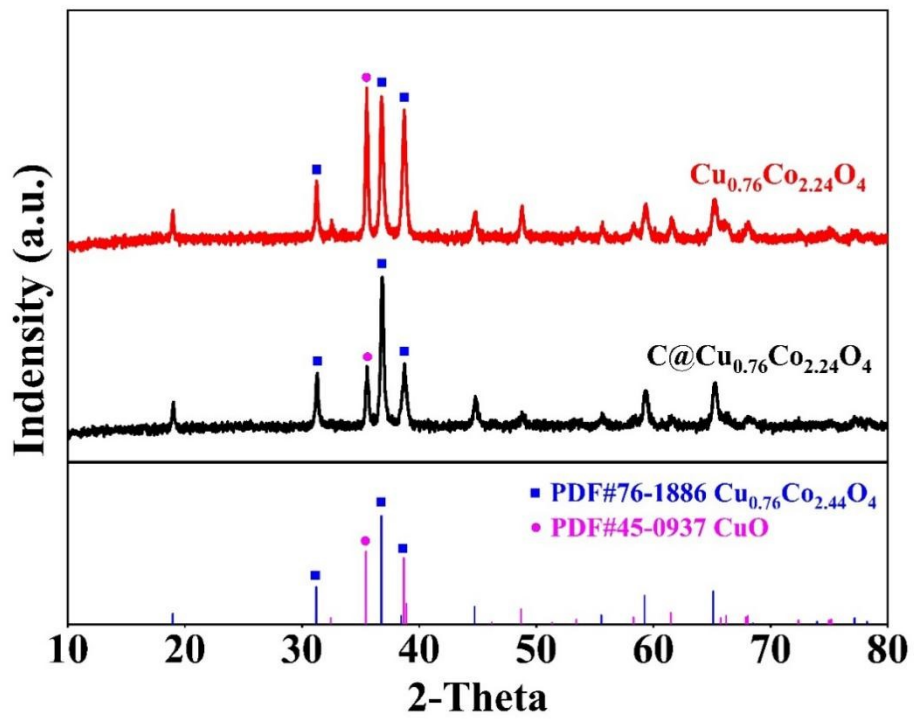


Figure S1 XRD patterns of $\text{C}@Cu_{0.76}\text{Co}_{2.24}\text{O}_4$ and $\text{Cu}_{0.76}\text{Co}_{2.24}\text{O}_4$

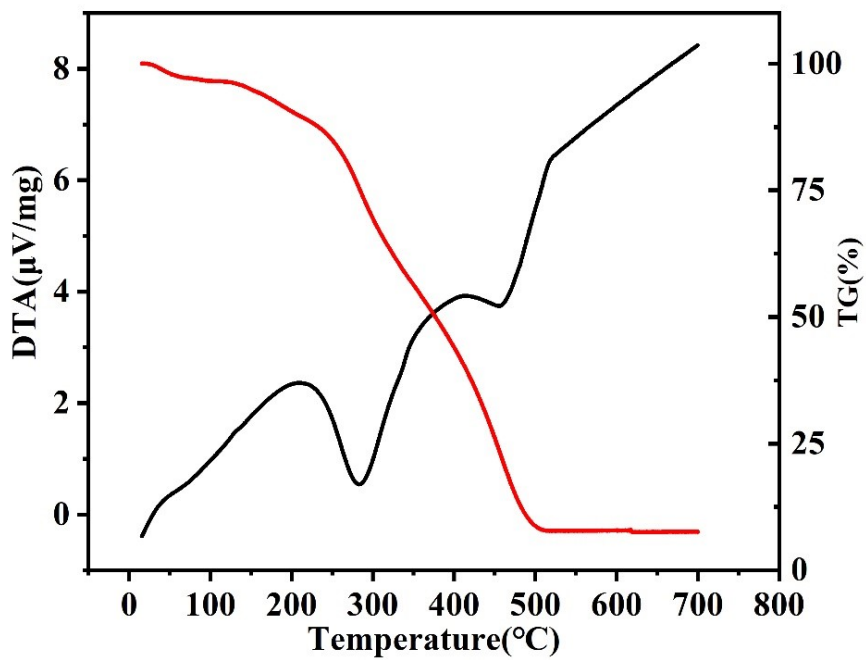


Figure S2 The thermal weight of a carbon sphere.

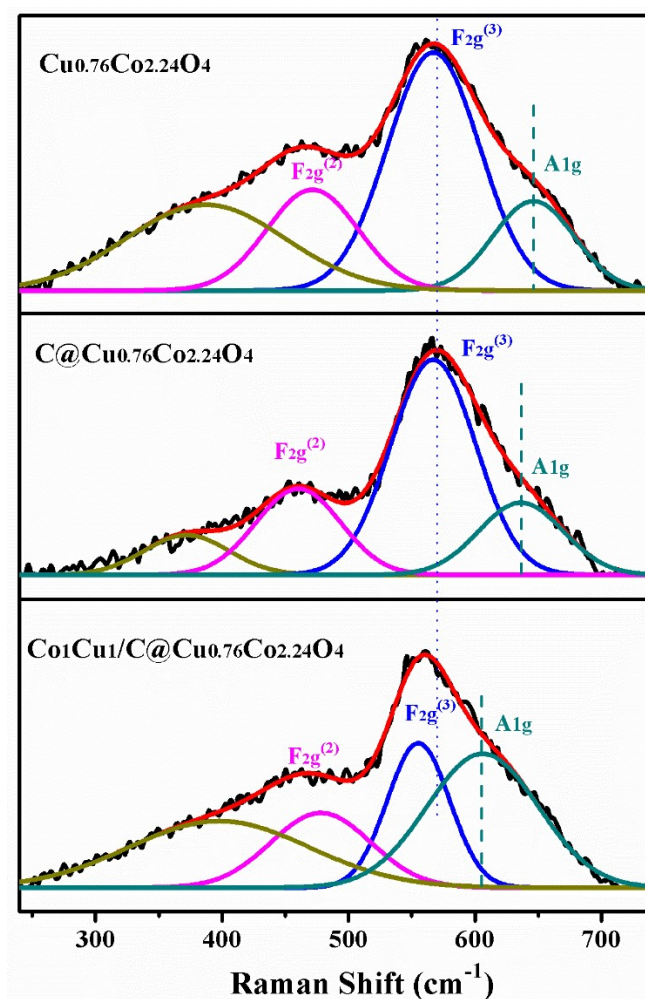


Figure S3 The Raman spectra.

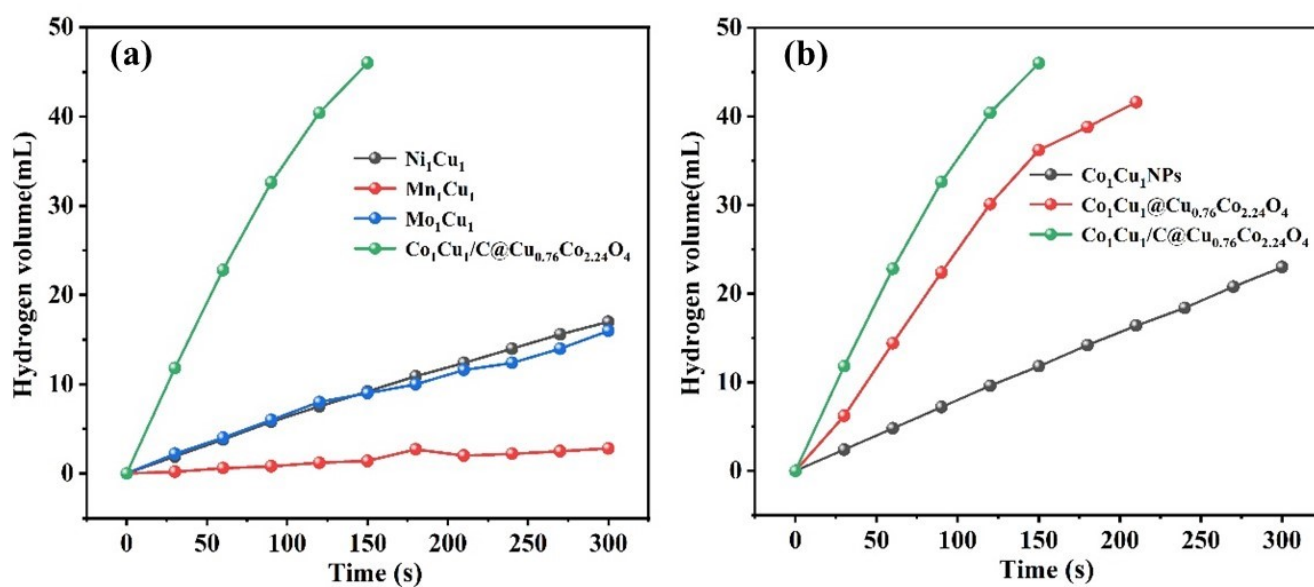


Figure S4 (a) Hydrolysis of AB catalyzed by different non noble metal catalysts; (b) Hydrolysis of AB catalyzed by $\text{Co}_1\text{Cu}_1\text{NPs}$, $\text{Co}_1\text{Cu}_1@Cu_{0.76}Co_{2.24}O_4$ and $\text{Co}_1\text{Cu}_1/\text{C}@Cu_{0.76}Co_{2.24}O_4$.

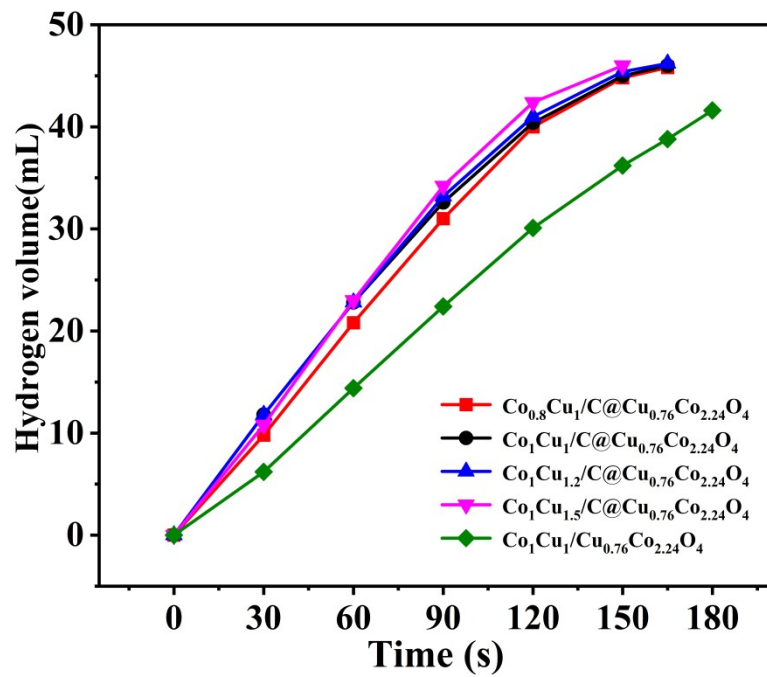


Figure S5 Hydrolysis of AB catalyzed by different ratio of Co/Cu in catalysts