

Supporting information

Boosted photothermal hydrogenation of acetylene on an efficient Au-Fe alloy catalyst

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Supplementary Methods

Materials

Reagents. Chloroauric acid (>99.9%), Chloroform, Ferrous chloride, Ferrous nitrate, ammonia and ethanol were purchased by Sinopharm (China). Chloroform and carbon black were bought from Aladdin. All the chemicals were used without further purification.

Catalyst preparation

Synthesis of 1 wt% Au-Fe/C catalyst by the impregnation method in water.

4.2 mg $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$ and 14.4 mg $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ were dissolved into 20 mL deionized water with stirring for 30 min. 0.4 g carbon black was synthesized before being dropped into the solution and then stirred for 8 h until both gold and ferrum were fully impregnated on the carrier with natural drying under room temperature. The obtained Au-Fe/C catalyst was heated to 873 K at 5 K / min in 5 vol. % H_2 / Ar atmosphere and calcining at 873 K for 4 h to obtain the reduced state catalysts. The loading amounts of gold and ferrum were determined by the ICP-OES instrument. The error between the drug dosage and the real loading did not exceed 3%.assist

Synthesis of 1 wt% Au /C, Fe/C, and Au-Fe/C catalysts in chloroform solution. As the typical synthesis of Au-Fe/C catalyst in the chloroform solution, 4.2 mg $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$ and 7.1 mg $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ were dissolved into 80 mL of chloroform to stir for 3 h. 0.4 g carbon black was added into the solution and then stirred for 2 h to perform sufficient loading. The mixture was filtered under vacuum condition and washed three times with 20 mL chloroform. The obtained catalysts were transferred into the tube furnace and reduced in H_2/Ar atmosphere at 673 K for 4 h to obtain the reduced state of catalysts. The loading amounts of gold and ferrum were determined using the ICP-OES instrument. The error between the drug dosage and the real loading did not exceed 3%.

Catalytic evaluation

Catalytic experiments. The performance of the catalyst was tested on a PFD-5000 photothermal fixed-bed reactor at standard atmospheric pressure (101kPa). Immersion of a high-pressure Xe lamp ($450 \text{ mW} \cdot \text{cm}^{-2}$) into this suspended system to

irradiate with the help of a visible light beam ($\lambda > 250$ nm) under the thermal process. 1000 mg catalysts and 2.0 g of quartz sand were mixed and then uniformly dispersed as a thin layer into the reactor. The catalyst was pretreated under flow of 5 vol.% H₂/Ar (20 mL min⁻¹) at 200 °C for 30 min, then cooled to room temperature. Subsequently, a gas mixture containing 1.0 vol.% C₂H₂, 20.0 vol.% H₂, 20.0 vol.% C₂H₄ and 59.0 vol.% Ar was introduced into the reactor at a space velocity of 1200 mL h⁻¹.g⁻¹, which was regulated by mass flow controllers. When the temperature in the reactor reached the preset temperature and stabilized for 20 min, take the product to the end of the reactor with the on-line collection before the upcoming examination. The gas products were analyzed by GC9790 gas chromatograph of Zhejiang Fuli Analytical Instrument Co., Ltd. C₂H₄ and C₂H₆ were the only C₂ products and oligomers formed could be ignored.

Acetylene conversion and selectivity to ethylene were calculated as follows:

$$\text{Conversion} = \frac{C_2H_2(\text{in}) - C_2H_2(\text{out})}{C_2H_2(\text{in})} \times 100\% \quad (1)$$

$$\text{Selectivity} = \left[1 - \frac{C_2H_6(\text{out}) - C_2H_6(\text{in})}{C_2H_2(\text{in}) - C_2H_2(\text{out})} \right] \times 100\% \quad (2)$$

Characterization of catalysts

X-ray diffraction analysis (XRD) was carried out on the Ultima IV diffractometer of RIGAKU company, using K_α ray from the Cu target, and receiving slit λ at 0.15406 nm. The operating voltage is set at 40 kV, along with the operating current at 30 mA. The scanning range is 30 ~ 50 °, and the scanning rate is 5° / min. The transmission electron microscope (TEM) analysis was carried out on the Titan G280-200 ChemiSTEM of FEI company, the acceleration voltage of which was 200 kV. Photoelectron spectroscopy characterization was carried out on the X-ray photoelectron spectrometer (XPS) of Thermo Fisher escalab250xi. After taking the 284.6 eV as the

standard C1s peak to correct the carbon balance, the atomic valence between gold and ferrum atoms supported on the catalyst surface was analyzed, and peaks were separated by the XPS peak software.

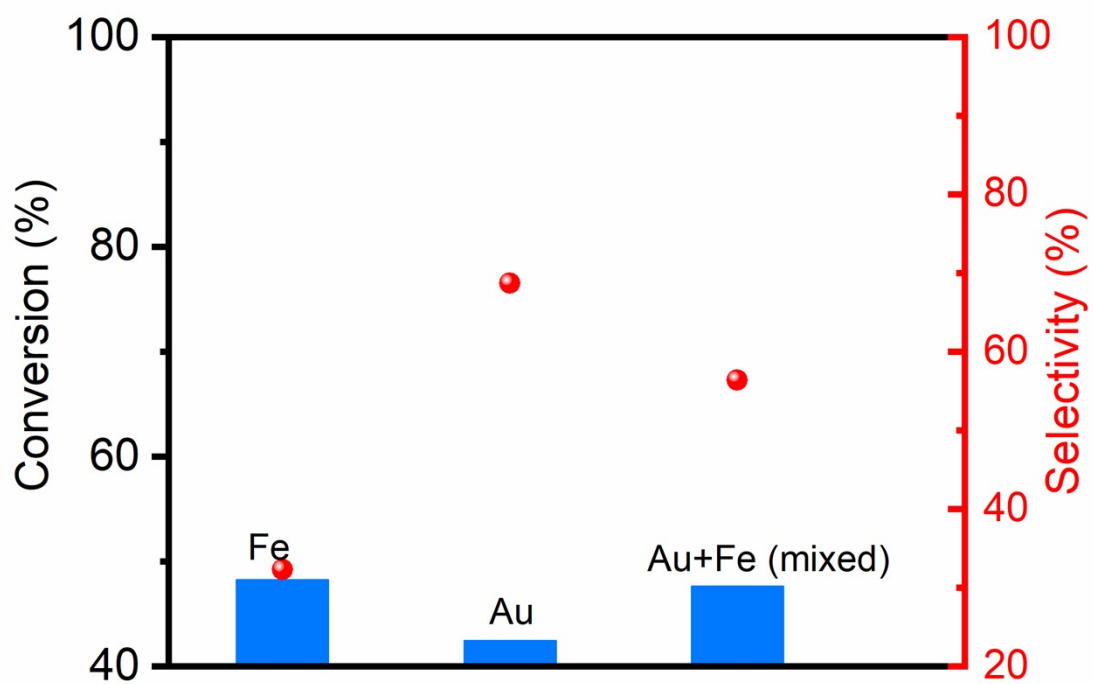


Figure S1 Conversion and selectivity of 200 mg mixed catalyst (1:1) for Au/C and Fe/C in the photothermal hydrogenation of acetylene.

Reacrants	Selectivity (%)		Maximum conversion (%)
	Au-Fe-water	Au-Fe-cholorform	
acetylene	83.5	97.5	98.4
propyne	78.3	96.9	96.6
propadiene	76.2	97.3	97.3
1-butylene	82.7	94.6	94.5
2-butylene	71.4	92.1	95.2

Table S1 Conversions and selectivities of hydrogenation for various olefins. All the catalysts masses were 1000 mg and in all cases, the reaction temperatures were at 130 °C and the selectivities are corresponded for the total olefin compounds excluding alkanes.

Catalytic performance				
Composition	Conversion (%)	Selectivity (%)	Temperature (°C)	Reference
Au/SiO₂	97	96	210	1
Au/CeO₂	85	100	300	2
Au-Ni	36	99	64	3
Au/ZnO	13.1	76.7	150	4
Au/TiO₂-C	100	80	250	5
Au-Ag/SiO₂	75	99	300	6
Au/CeO₂	>60	94	250	7
Au/MgO-Al₂O₃	45	100	250	8
AuFe/C	98.4	97.5	130	Present study

Table S2 Comparison of different Au-based catalysts in the photothermal/thermal hydrogenation of acetylene.

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