An ultra-high H₂S-resistant gold-based imidazolium ionic liquid catalyst for acetylene hydrochlorination

Supporting Information

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 Table S1 Average content of major impurities in acetylene

Impurity	H_2S	DVS ^a	PH_3	VA ^b
ppm	250	700	400	400

^a Divinyl Sulfide ^b Vinyl Acetyl

Element	Weight %	Atomic %
С(К)	98.71	99.78
S(K)	0.35	0.13
CI(K)	0.07	0.02
Au(L)	0.85	0.05

Table S2 EDS-mapping Quantification Results of Au/AC-S catalyst.



Fig. S1. TEM images of (a) Au/AC-Used, (b) and (c) Au/AC-S.



Figure S2. EDS spectrum source data of (a) Au/AC (b) Au/AC-S (c) Au-IL/AC (d) Au-IL/AC-S.



Figure S3. (a) FT-IR spectrum of fresh and H_2S -treated IL and Au-IL (b) S 2p spectral line of the Au-IL/AC catalyst treated with H_2S at 180 °C for different time



Figure S4. Schematic diagram of the hydrochlorination reactor.

Adsorptivity of H₂S in the Au-IL/AC is determined by referring to the methods in the relevant literature¹⁻², which was depicted in Figure S5. Figure S6 and S7 show the adsorption quantity and fit linear of H₂S in Au-IL/AC at 30 °C (303K) and 180 °C (453K), respectively. The relationship curve between *q* (adsorption quantity, mg_{H2S}/g_{IL}) and *C_e* (equilibrium concentration, mg_{H2S}/L_{IL}) conforms to *Langmuir* adsorption isotherm. *Langmuir* adsorption isotherm is the most commonly used equation to describe the adsorption isotherm. The commonly used linear form of *Langmuir* adsorption isotherm can be described by the following equation:

$$\frac{C_e}{q_e} = \frac{1}{K \cdot q_m} + \frac{1}{q_m} C_e$$

Where: C_e is equilibrium concentration, mg_{H2S}/L_{IL} ; q_e is equilibrium adsorption quantity, mg_{H2S}/g_{IL} ; K is equilibrium constant, L/mg; q_m is maximal equilibrium adsorption quantity, mg_{H2S}/g_{IL} .

It can be seen that C_e/q_e has a linear relationship with C_e , as shown in Figure S6 and S7 (red dashed line). The adsorption equilibrium constant (*K*) at 30 °C (303K) and 160 °C (303K) calculated from the slope and intercept of the straight line is 0.83 and 0.24 L/mg, respectively.



Figure S5. Adsorption isotherm at 30 °C (303K) and 180 °C (453K).



Figure S6. Adsorption isotherm and linear fit using Langmuir model at 30 °C (303K).



Figure S7. Adsorption isotherm and linear fit using Langmuir model at 180 °C (453K).

To further investigate the influence of IL addition, we performed the Au-IL/AC catalyst at high temperature (180 °C) and high GHSV (740h⁻¹), Au/AC catalyst was used for comparison. The result was shown in Figure S8. From Figure S8b, we can see that Au-IL/AC catalyst exhibits good stability and catalytic activity in the presence of H₂S, which almost consistent with H₂S-free test. As for Au/AC catalyst, the presence of H₂S during the reaction extremely poisoning the active site, because the initial activity and catalytic stability were greatly decreased (Figure S8a). Figure S9 displays the catalytic performance of Au-IL/AC catalyst at higher reaction temperature (200 °C), we can see that the catalyst still performed a good stability with the presence of H₂S. Thus it is very clear that the addition of IL can slow down the deactivation process.



Figure S8. Catalytic performance of (a) 1% Au/AC and (b) 1% Au-20%IL/AC at 740 h^{-1} and 180 °C with and without $H_2S.$



Figure S9. Catalytic performance of 1% Au-20%IL/AC at 740 $h^{\text{-1}}$ and 200 °C with and without $H_2S.$

Notes and references

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