Ligand coordination approach for high reaction stability of an Au-Cu bimetallic carbon-based catalyst in acetylene hydrochlorination process

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Supplementary Information

Table S1 The development of PVC industry in China in the last 10 years, unit: 10^4 t.

Year	Production Capacity	Yield			Consumption
		All	Acetylene Method	Ethylene Method	
2004	676	503.2	301	198	701.3
2005	823	668.2	420	239	820.05
2006	1122	823.8	569	245	918.09
2007	1341	971.7	710	256	1026.76
2008	1650	822.5	555	259	830.92
2009	1764	798	527	261	1026.9
2010	2050	1188	838	342	1083.5
2011	2238	1295	887	399	1298
2012	2303	1595	1218	374	1698
2013	2468	1790	—	—	1915

Table S2 Energy calculation results for each optimized species in Fig. 9 and Fig. S7, energy unit: kJ/mol.

Au system		Au/TCCA system		Au/CA system		Au/Melamine system	
Species	Energy	Species	Energy	Species	Energy	Species	Energy
Au_2Cl_6	-1902288.12	Au_2Cl_5-TCCA	-2796587.07	Au_2Cl_5-CA	-2220033.31	Au_2Cl_5-M	-2182410.92
C_2H_2	-48522.58	C_2H_2	-48522.58	C_2H_2	-48522.58	C_2H_2	-48522.58
Au_2Cl_6-C_2H_2	-1951273.67	Au_2Cl_5-TCCA-C_2H_2	-2844539.29	Au_2Cl_5-CA-C_2H_2	-2268373.21	Au_2Cl_5-M-C_2H_2	-2230794.24
E_{ads}	62.97	E_{ads}	-570.35	E_{ads}	182.68	E_{ads}	139.25

*Subscript ads denotes for adsorption which was calculated by E(reactant)-E(complex).

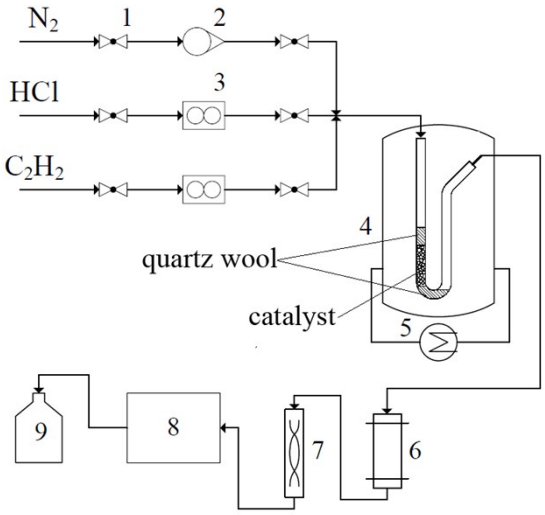

Fig. S1. Diagram of the experimental equipment (1) Ball valve; (2) Rotor flowmeter; (3) Mass flowmeter; (4) Furnace; (5) Heater; (6) Condenser; (7) Dryer; (8) Gas chromatography; (9) Exhausted gas absorption bottle.

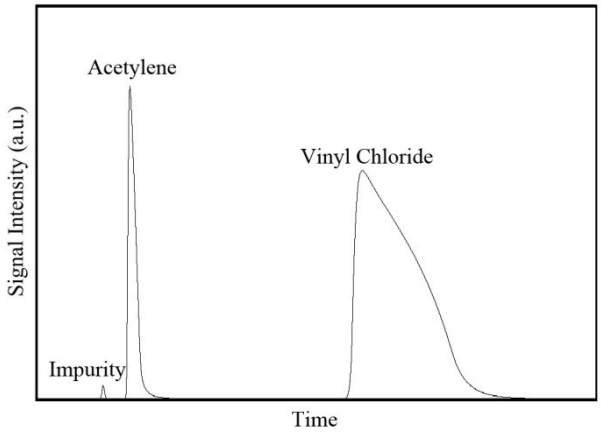

Fig. S2. Typical chromatogram during hydrochlorination reaction.

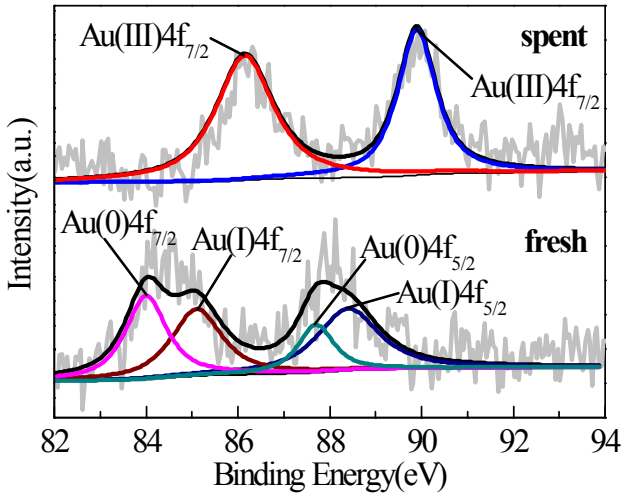

Fig. S3. XPS spectrum for Au/Cu/TCCA system, Au content 0.25wt%, Au:Cu:TCCA=1:5:20 (mole ratio).

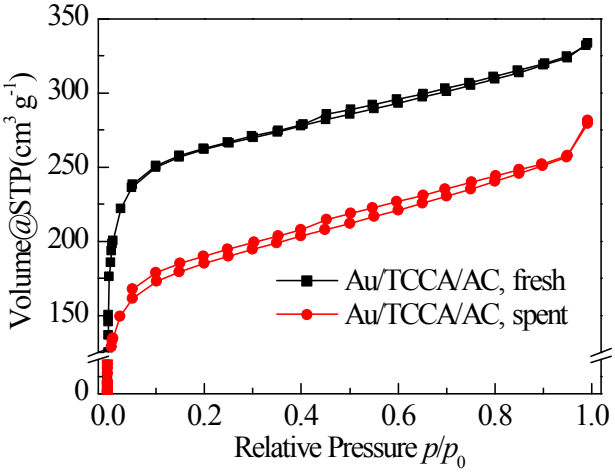

Fig. S4. Typical Ar adsorption/desorption isotherm for Au/TCCA/AC catalysts, Au content 0.25wt%, Au:TCCA=1:20 (mole ratio).

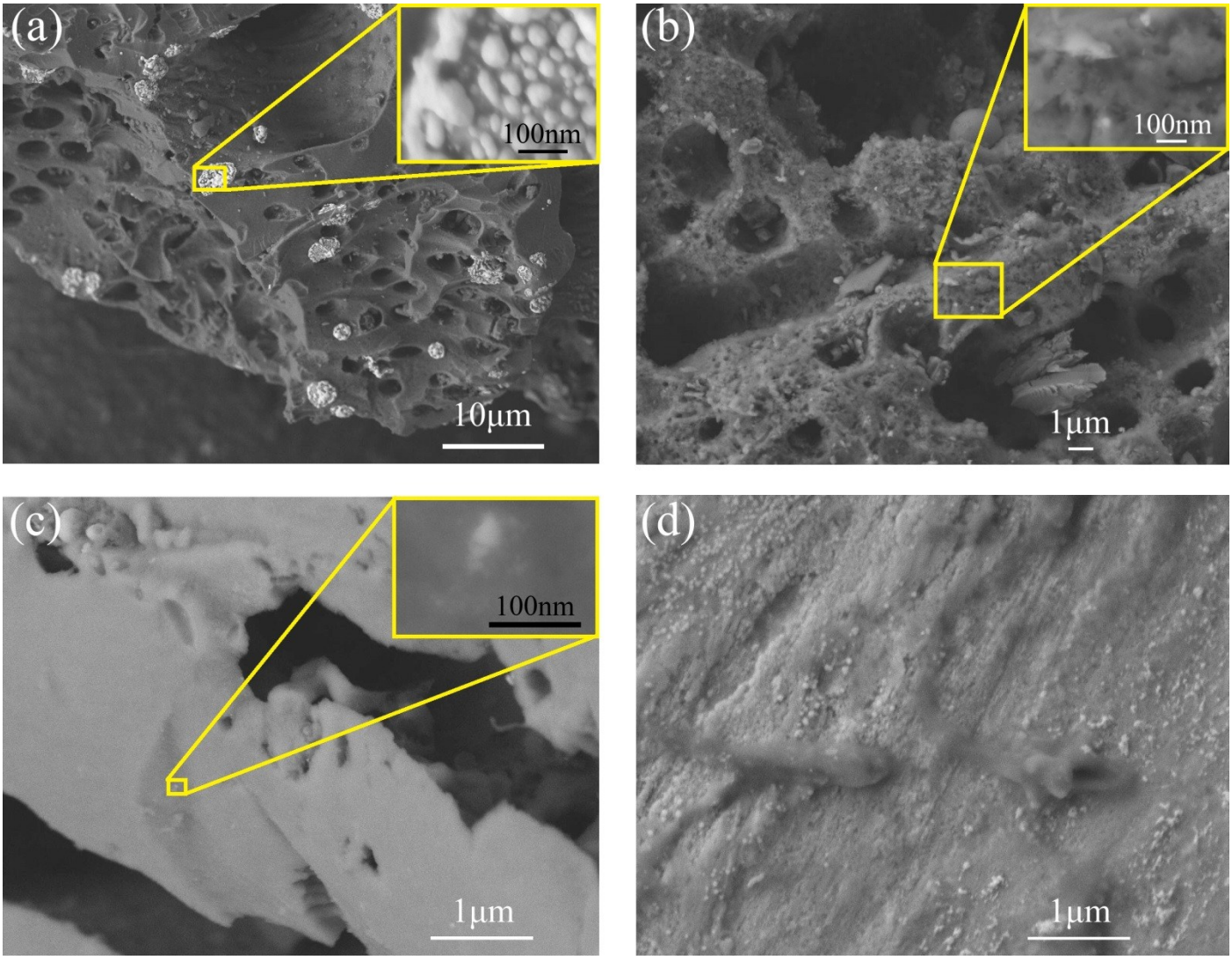

Fig. S5 SEM images of Au/TCCA/AC catalysts, (a)no ligand, (b)Au:TCCA=1:8, (c)Au:TCCA=1:20, (d)Au:TCCA=1:40, Au content 0.5 wt%.

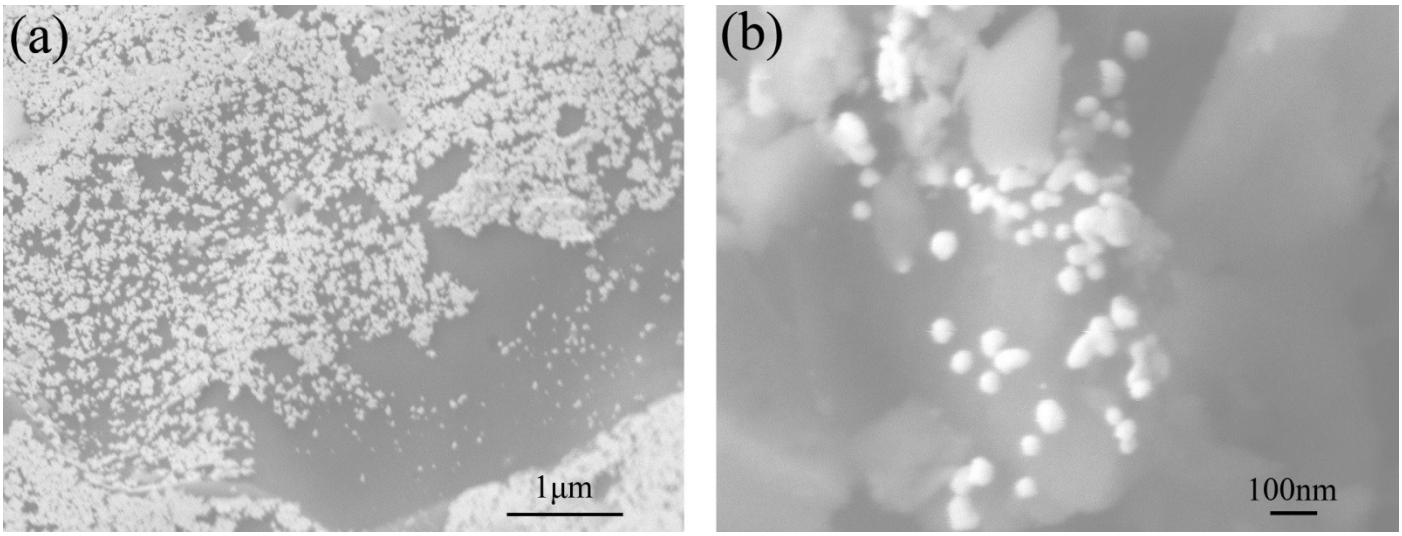

Fig. S6 SEM image of $Au/Na_2S_2O_3/AC$ catalyst, Au content 0.25 wt%.