

Ag- and Cu-Promoted Mesoporous Ta-SiO₂ Catalysts Prepared by Non-Hydrolytic Sol-Gel for the Conversion of Ethanol to Butadiene

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Table S1. Textural properties (N₂-physisorption) for catalysts used in catalytic study.

Sample	S _{BET} (m ² g ⁻¹)	V _p (cm ³ g ⁻¹) ^a	V _μ (cm ³ g ⁻¹) ^b	D _p (nm) ^c
4TaSi ^{NHSG} -5Ag	490	0.43	0.08	3.5
2TaSi ^{NHSG} -2Ag	670	0.58	0.11	3.5
2TaSi ^{NHSG} -5Ag	580	0.55	0.08	3.8
2Ta ^{IMP} Si-5Ag	n.m	n.m	n.m	n.m
2TaSi5Ag ^{NHSG}	710	0.89	0.08	5.0
2TaSi5Cu ^{NHSG}	640	0.60	0.07	3.8

^a Pore volume at P/P₀=0.98; ^b Micropore volume at P/P₀=0.98; ^c Calculated as 4V_p/S_{BET}.

Table S2. Synthesis of Si-Ta binary oxides – amounts of precursors and surfactant.

Sample	Si(OAc) ₄ mass (g)	Ta(NMe ₂) ₅ mass (g)	F127 mass (g)
4Ta ^{NHSG}	7.0927	0.1796	3.6331
2Ta ^{NHSG} ^a	10.6386	0.1346	5.4475
Si ^{NHSG}	7.0930	0.0035	3.6308

^a Quantity x1.5, amount of solvent was adjusted accordingly.

Table S3. Impregnation of silver – amounts of catalyst and Ag salt used.

Sample	Impregnated mass (g)	AgNO ₃ mass (g)
4Ta ^{NHSG} -2Ag	1.0002	0.0321
4Ta ^{NHSG} -5Ag	1.0026	0.0841
2Ta ^{NHSG} -2Ag	1.0017	0.0325
2Ta ^{NHSG} -5Ag	1.0009	0.0845

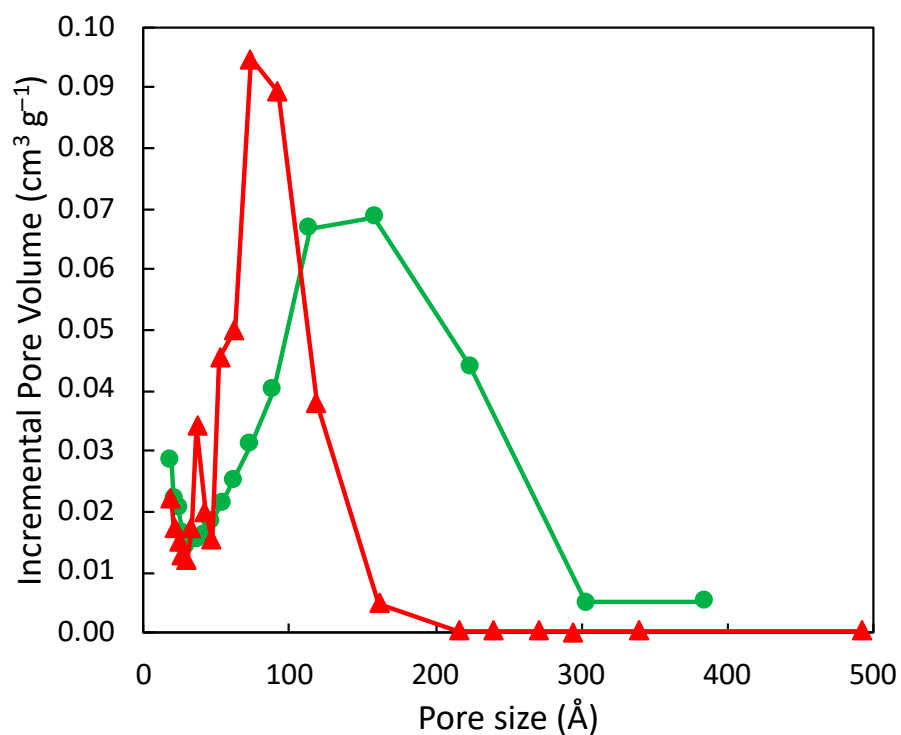


Figure S1. Pore size distribution in 4TaSiNHSG-2Ag by the BJH model (from the adsorption curve in green ●; from the desorption curve in red ▲).

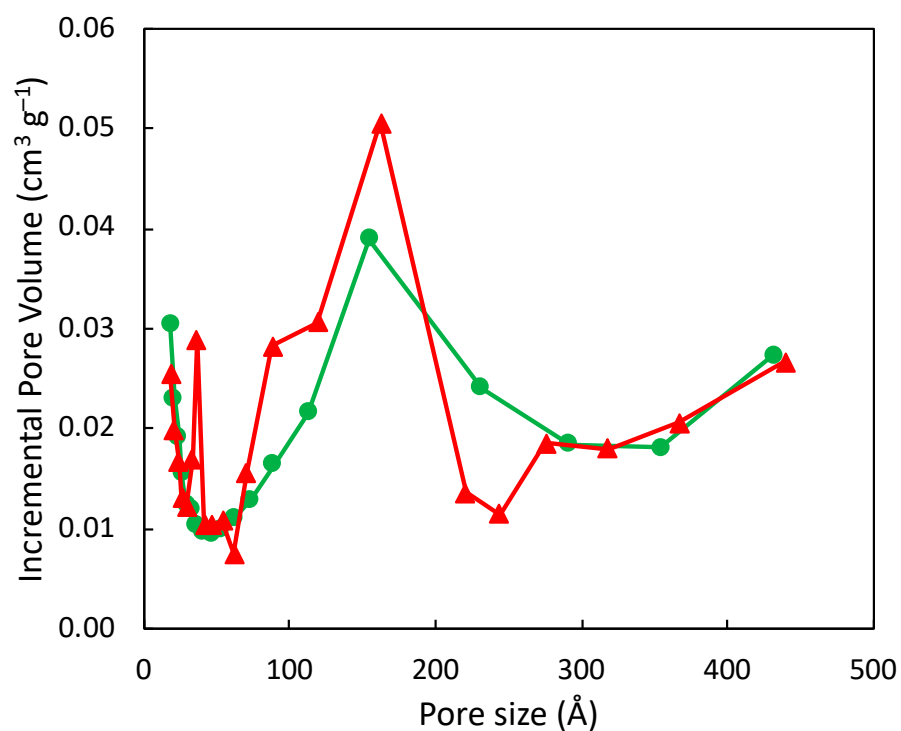


Figure S2. Pore size distribution in 4TaIMP-Si-2Ag by the BJH model (from the adsorption curve in green ●; from the desorption curve in red ▲).

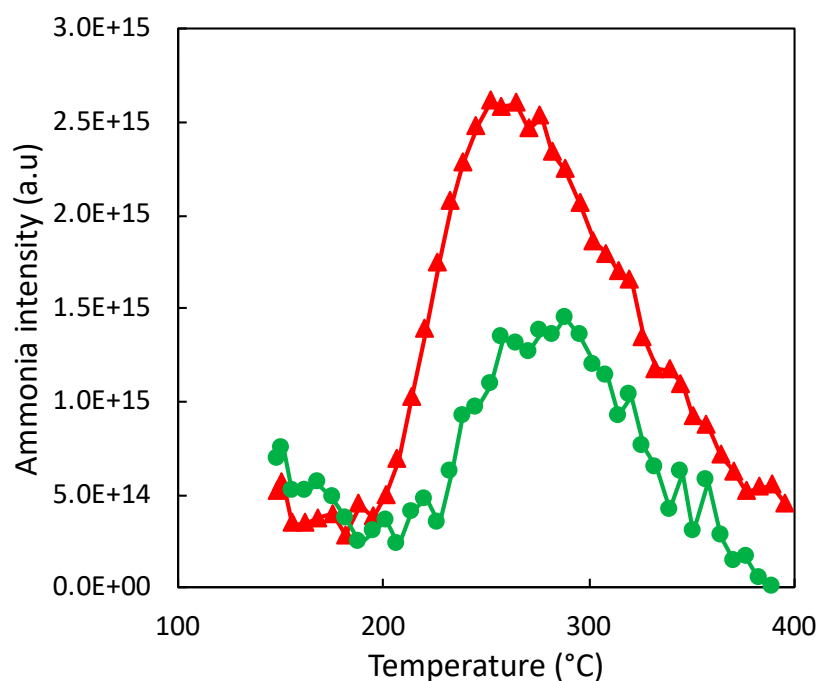


Figure S3. Ammonia desorption profiles of 4TaSiNHSG-2Ag (red ▲) and 4TaIMP-Si-2Ag (green ●).

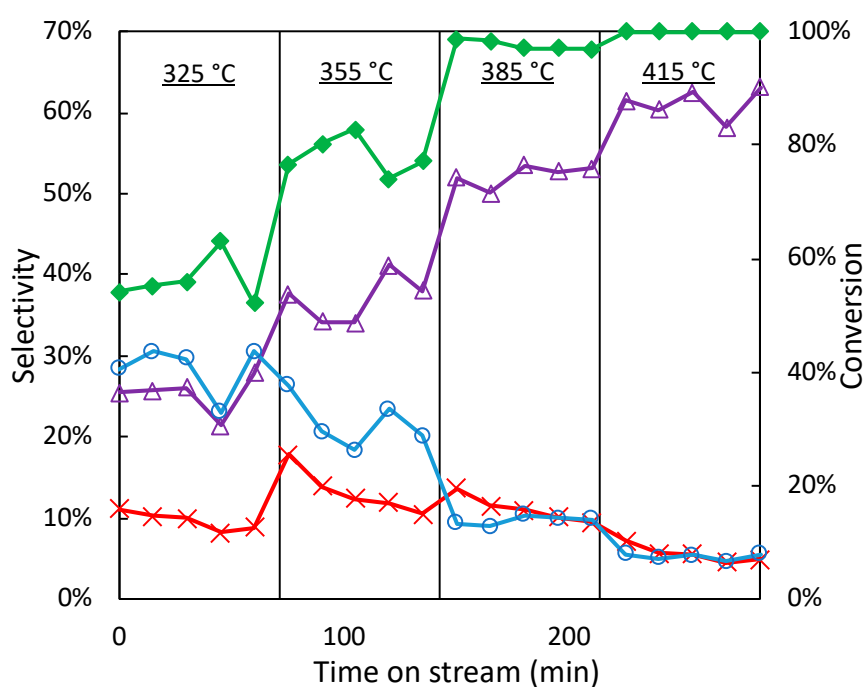


Figure S4. Evolution of ethanol conversion (green ◇), butadiene selectivity (red ×), acetaldehyde selectivity (blue ○) and ethylene selectivity (purple △) over time for all tested temperatures for 4TaSiNHSG-2Ag. Note: the spent catalyst has a brownish color, indicative of coke formation. At 385 °C and 415 °C, the carbon balance is incomplete (at lower temperature, it accounts for >95%).

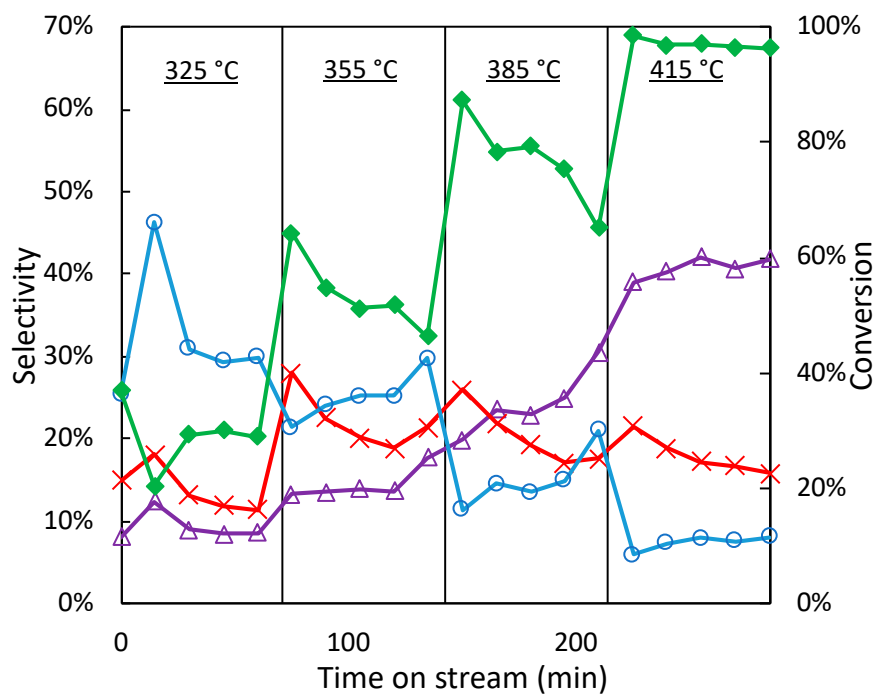


Figure S5. Evolution of ethanol conversion (green $\diamond$), butadiene selectivity (red $\times$), acetaldehyde selectivity (blue $\circ$) and ethylene selectivity (purple Δ) over time for all tested temperatures for 4Ta₁₀MPSi 2Ag.

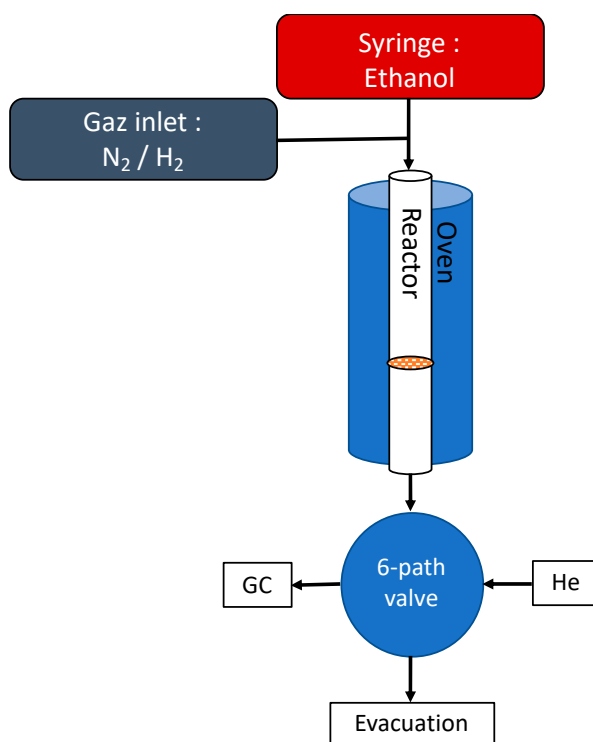


Figure S6. Schematic view of the catalytic setup.