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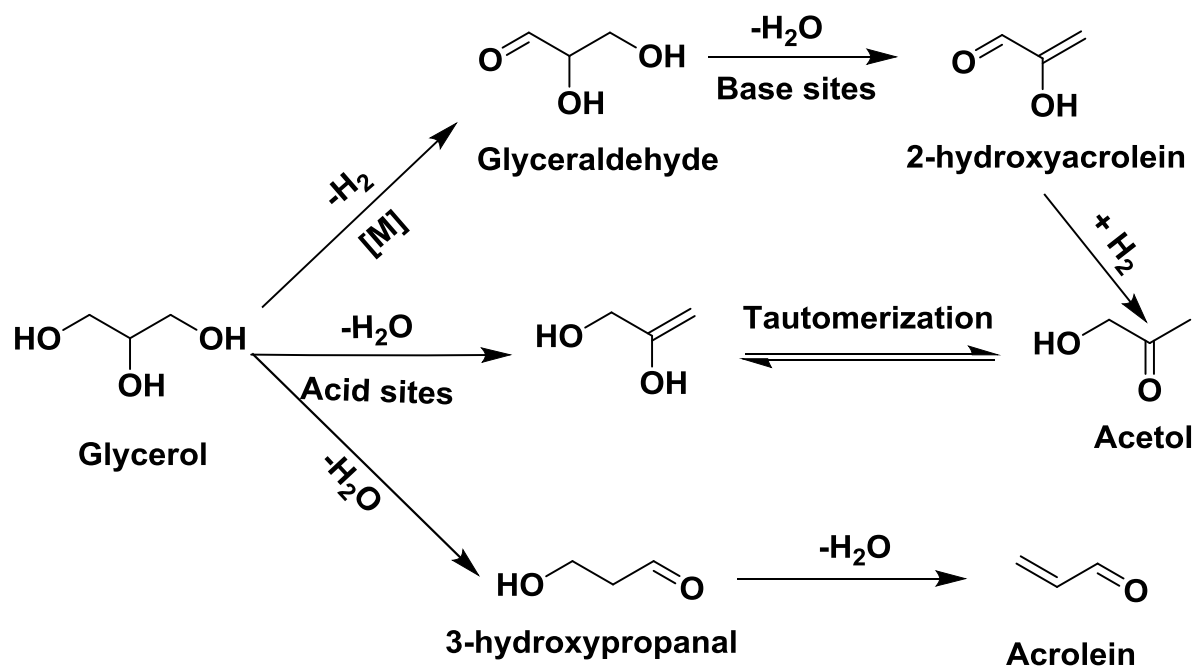
Active sites in modified copper based catalysts for selective liquid phase dehydration of aqueous glycerol to acetol

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Experimental

Powder X-ray diffraction of all the samples were carried out in a PANalytical X'pert Pro diffractometer using Cu K α (1.5418 Å) radiations with a Ni filter and a X'celerator solid state detector . The crystallite size was determined by Scherrer equation.

$$D = k\lambda/\beta \cos \theta$$



Scheme 1. Various glycerol dehydration pathways depending on acid and base sites of the catalysts.

Table 1 Crystallite size of different activated (A) and recovered (R) copper catalysts

Catalyst	Crystallite size of Cu (nm)
ACu:Ba	-
ACu:Mg	5.5
ACu:Zr	38.8
ACu:Zn	-
ACu:Al	14.4
ANMT006	24.4
RCu:Ba	50.2
RCu:Mg	27.5
RCu:Zr	38.8
RCu:Zn	56.9
RCu:Al	35.6

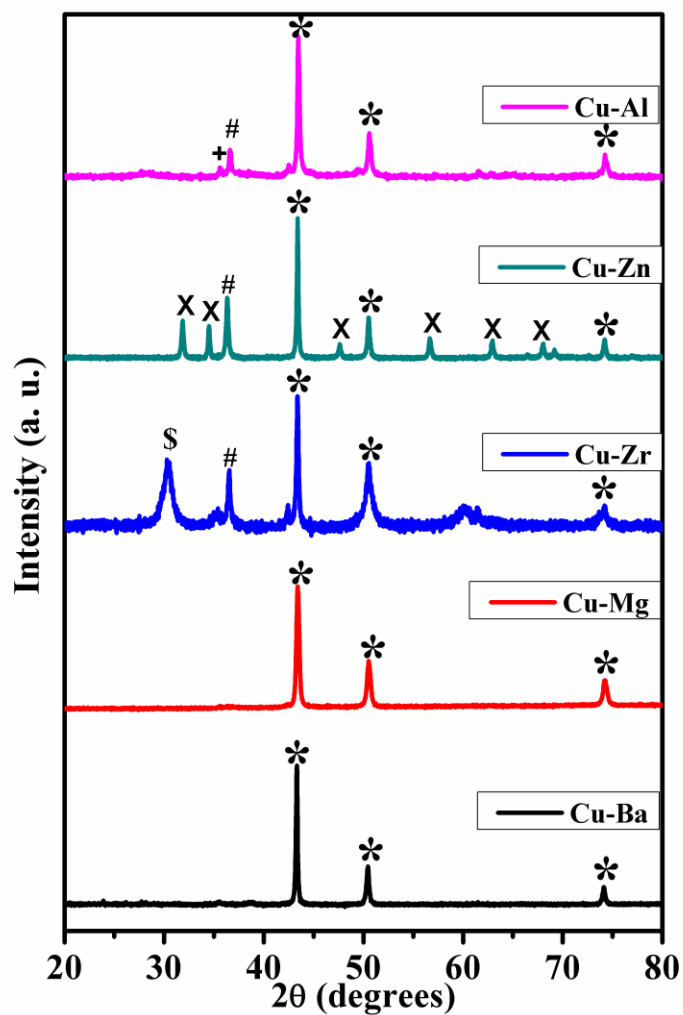


Fig. 1 XRD patterns of different recovered copper catalysts. (*) Cu^0 , (#) Cu_2O , (+) CuO , (\$) $t\text{-ZrO}_2$, (X) ZnO .

Table 2 NH₃-TPD results of different copper catalysts

Catalyst	Temperature at maximum (°C)	NH ₃ desorbed (mL g ⁻¹)
Cu-Ba	334	4.05
Cu-Mg	325	45.71
Cu-Zr	564	3.5
	630	5.9
Cu-Zn	302	7.52
Cu-Al	564	3.2
	630	6.31

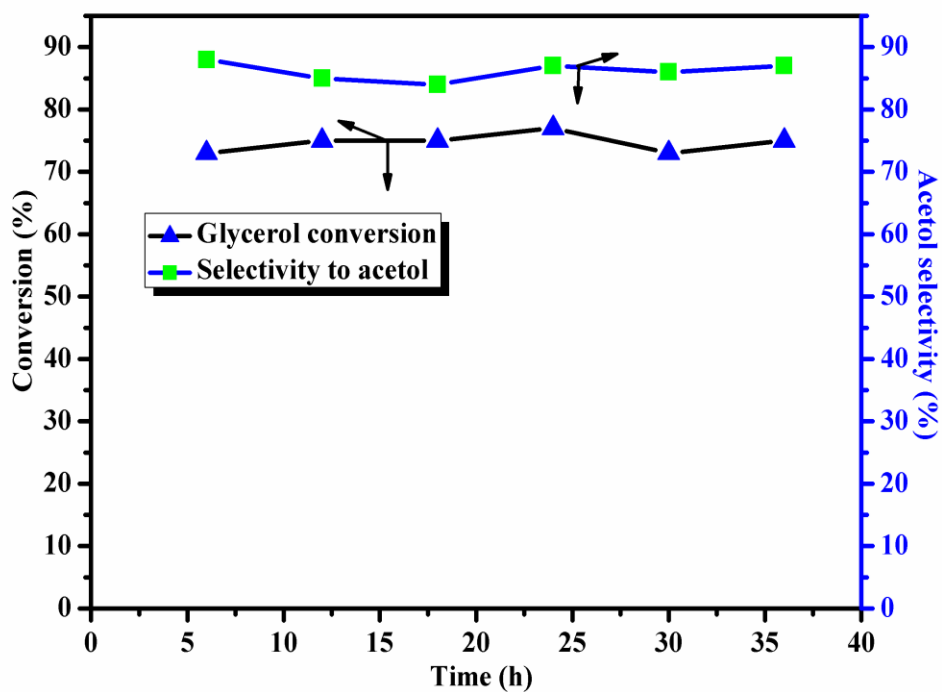


Fig. 2 Time on stream activity of Cu-Al catalyst.

Reaction conditions: 20 wt% glycerol aqueous solution , without N₂ pressure, GHSV = 500 h⁻¹,

LHSV = 1.53 h⁻¹.