Supplementary material to:

J. Valand, V.D.B.C. Dasireddy, A.S. Mahomed and H.B. Friedrich,

Transition Metal Oxide Supported on Alumina Catalysts: A Comparative Study for the Hydrogenation of Octanal

S. Afr. J. Chem., 2018, **71**, 135–139.

Supplementary Data

Chemisorption analysis (Micromeritics ASAP 2020):

Metal dispersion (%):

$$\%\, M_{disp} = \frac{100\% \times 100\%}{22414^{*}} \times \frac{\mathrm{V} \times \mathrm{SFcalc}}{\%\mathrm{Weight}/\mathrm{Watomic}}$$

Where,

$\%M_{DISP}$ is metal dispersion (%)

V in cm^3/g, STP, is volume intercept derived from the best line fit to the volume differences between the selected points of the first analysis and the repeat analysis. If $\%M_{Disp}$ is being calculated from analysis data, then V is the volume intercept derived from the best line fit of the points selected for line fit. If $M\%_{Disp}$ is being calculated from difference data, then V is V_{Diff}.

SF_{Calc} is the calculated stoichiometry factor

The calculated stoichiometry factor is a weighted average. It is dependent on both the individual stoichiometry factor and the number of moles of each active metal

%Weight is % of sample weight for metal

W_{Atomic} is atomic weight of metal (g/mole)

Metallic surface area:

The metallic surface area per gram of sample is the total active surface area available for interaction with the adsorbate and is calculated using the equation;

$$M_{sa} = \frac{6.023 \times 10^{23}}{22414^{*}} \times \mathrm{V} \times SF_{CALC} \times A_{AREA}$$

Where,

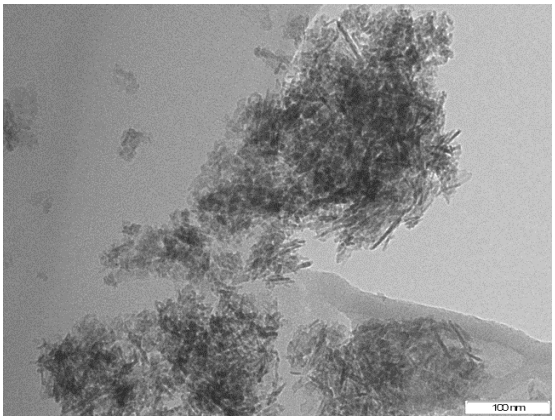
M_{sa} is the metallic surface area (m^2/g) of sample

V = (cm^3/g STP). If M_{sa} is being calculated from analysis data, then V is the volume intercept derived from the best line fit of the points selected for line fit. If M_{sa} is being calculated from difference data, then V is V_{Diff}.

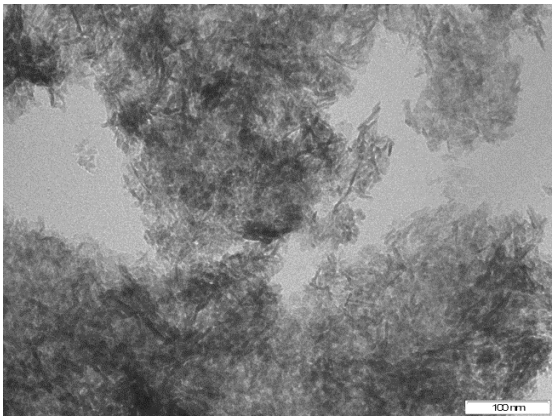
A_{AREA} is effective area of 1 active metal atom (m^2/atom)

SF_{CALC} is the calculated stoichiometry factor

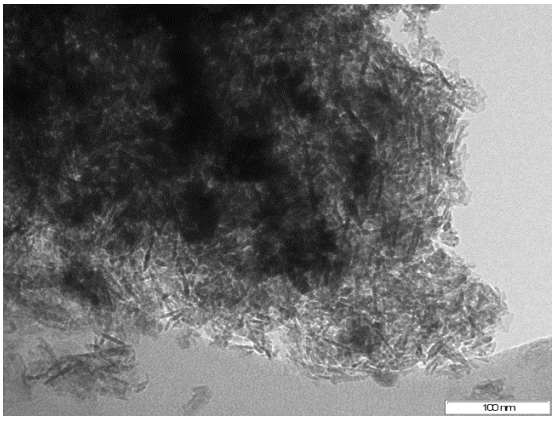
V_{DIFF} is difference in volume between the first analysis and the repeat analysis



(a)



(b)



(c)

Fig. S1. TEM images of (a) Cu-Al (b) Ni-Al and (c) Co-A1 catalysts.

Activation energy:

The Activation Energy (Ea) was calculated using the Arrhenius Equation:

$$k = Ze^{-E_a/RT}$$

Where Z (or A) is the pre-exponential factor, k is the rate constant, R is the gas constant (8.314 J/mol-K), T is the temperature in Kelvin. When lnk (rate constant) is plotted against the inverse of the temperature (kelvin), the slope is a straight line. The value of the slope (m) is equal to $-E_a/R$ where R is a constant equal to 8.314 J/mol-K. Z or A was determined from the intercept.

The activation energy in this study was calculated by using the rate constant (assuming first order reaction), calculated by the conversion of octanal obtained with an octanal to hydrogen molar ratio of 1:2. GHSV and LHSV were maintained at 460 h^{-1} and 18 h^{-1} respectively, at temperatures of 110 ºC, 150 ºC and 180 ºC.

Turn over number (TON):

Turn over number = (moles of octanal converted)/(moles of active sites per gram of catalyst) or mol g^{-1} .