

Supporting Information

for

Short-channel mesoporous SBA-15 silica modified by aluminum grafting as support for CoRu Fischer-Tropsch synthesis catalysts

Sophia Mohammadnasabomran,^a Carlos Márquez-Álvarez,^b Joaquín Pérez-Pariente,^{*b} and Agustín Martínez ^{*c}

^a School of Chemistry, College of Science, University of Tehran, Tehran, Iran.

^b Instituto de Catálisis y Petroleoquímica, ICP-CSIC, C/Marie Curie 2, 28049, Madrid, Spain.

^c Instituto de Tecnología Química, Universitat Politècnica de València – Consejo Superior de Investigaciones Científicas (UPV – CSIC), Avda. de los Naranjos s/n, 46022 Valencia, Spain.

* Corresponding authors: jperez@icp.csic.es (J. Pérez-Pariente); amart@itq.upv.es (A. Martínez).

Estimation of the contribution of Ru⁰ species to the overall FTS activity of CRLPS and CRALPS catalysts

The following assumptions were made to estimate the contribution of active Ru⁰ species to the overall FTS activity of CRLPS and CRALPS catalysts:

- a) Both Ru⁰ and Co⁰ active sites exhibit the same TOF [1].
- b) The dispersion of Ru⁰ species is 100%, which would correspond to the extreme situation where the contribution of Ru⁰ sites would be maximal.

Taking into account the above assumptions, the contribution of surface Ru⁰ species to the overall activity of our Ru-promoted Co catalysts could be estimated by simply considering the concentrations of accessible Co⁰ and Ru⁰ sites. Since we only know the total concentration of surface metal (Co⁰+Ru⁰) sites from the total H₂ uptake determined by H₂ chemisorption (Table 3), we can determine the H₂ uptake associated to Ru by considering 100% dispersion of Ru⁰ species. After subtracting this value from the total H₂ uptake, we can then recalculate the Co dispersion (D(Co)) assuming a chemisorption stoichiometry H:metal = 1:1 for both Co⁰ and Ru⁰. Thus, the concentration of surface Co⁰ and Ru⁰ sites can be determined from the metal contents (measured by ICP-OES) and metal dispersions, from which the % contribution of Ru⁰ sites to the total FTS activity (FT_{Ru}) can be directly estimated as:

$$FT_{Ru} (\%) = [Ru^0]_s / ([Co^0]_s + [Ru^0]_s) \cdot 100$$

where [Co⁰]_s and [Ru⁰]_s are the concentrations of surface Co⁰ and Ru⁰ sites, respectively.

The results of such calculations are compiled in Table S1 for our CRLPS and CRALPS catalysts.

Table S1. Estimation of the contribution of Ru⁰ sites to the total FTS activity (FT_{Ru}) of CRLPA and CRALPS catalysts.

Catalyst	Co (wt%)	Ru (wt%)	H ₂ uptake (μmol/g _{cat})		D(Co) (%)	[Co ⁰] _s (μmol/g _{cat})	[Ru ⁰] _s (μmol/g _{cat})	FT _{Ru} (%)	
			Total	Ru					Co
CRLPS	17.1	0.3	156	14.8	141.2	9.7	282.3	29.7	9.5
CRALPS	16.5	0.2	192	9.9	182.1	13.0	364.2	19.8	5.2

[1] E. Iglesia, S.L. Soled, R.A. Fiato, J. Catal. 137 (1992) 212.

Figure S1. Evolution of the CO conversion with time-on-stream (TOS) during period 1 (constant GHSV) and period 2 (constant CO conversion) for CRLPS and CRALPS catalysts. Reaction conditions: 220 °C, 2.0 MPa, H₂/CO molar ratio of 2.

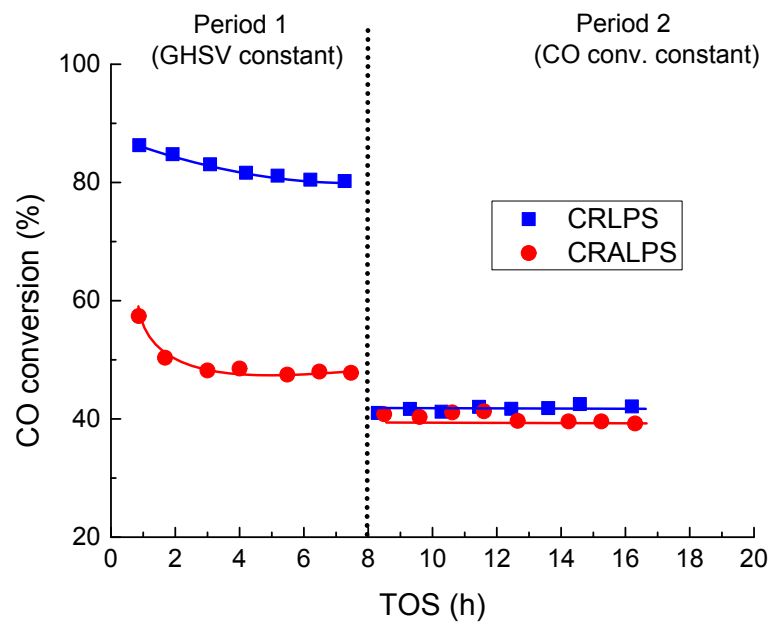


Figure S2. ASF distributions for CRLPS and CRALPS catalysts at constant CO conversion of ca. 40% (period 2). Reaction conditions: 220 °C, 2.0 MPa, and H₂/CO = 2.

