Supplementary materials

Tuning Ethanol Synthesis Pathways from Syngas: Nanosheet-Structured K-Doped Co-MoS_2 Catalysts and the Role of CVD Sulfidation

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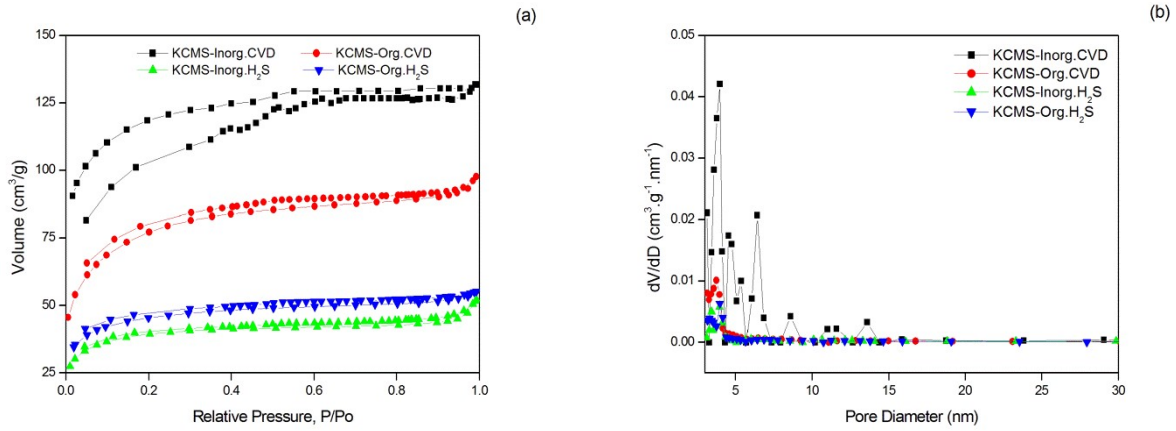


Figure S1. Textural characteristics of sulfided catalysts understudy: ***(a)*** N_2-adsorption isotherms; ***(b)*** Pore size distribution

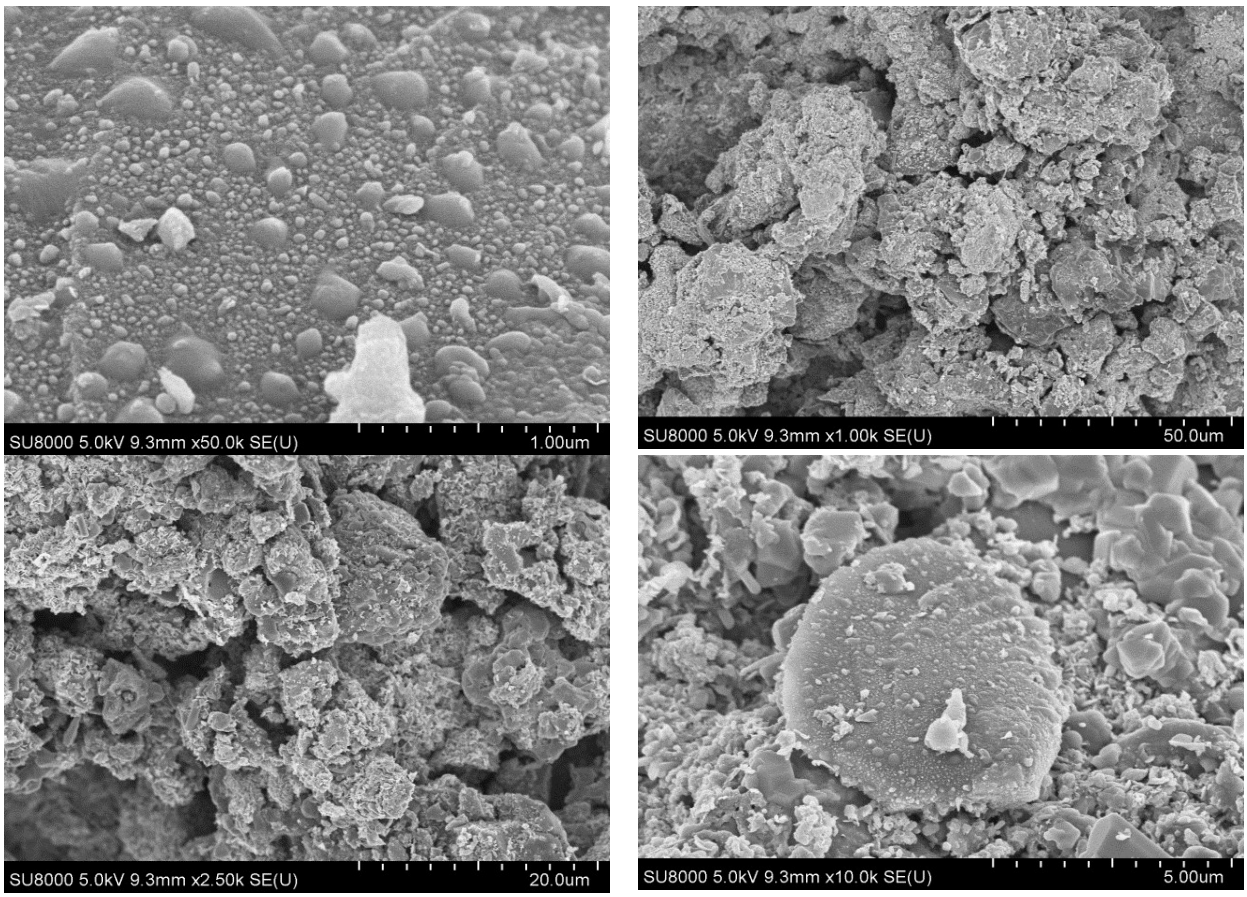


Figure S2. SEM micrographs of AJ-3 activated carbon support

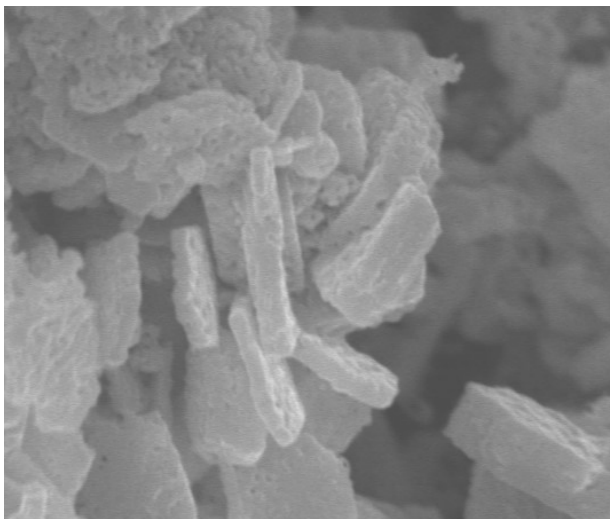


Figure S3. Additional SEM image of KCMS-Inorg.CVD

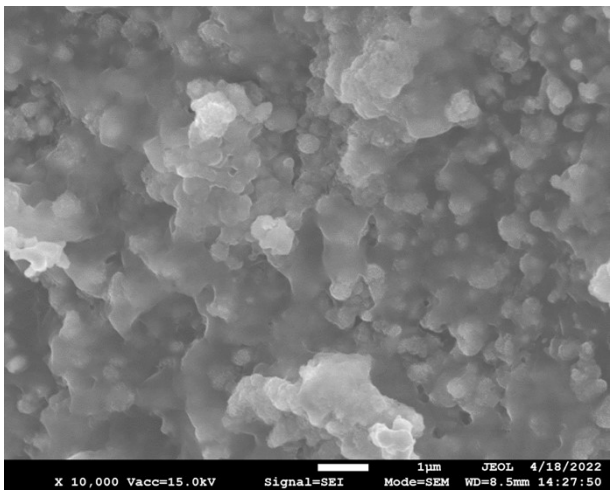
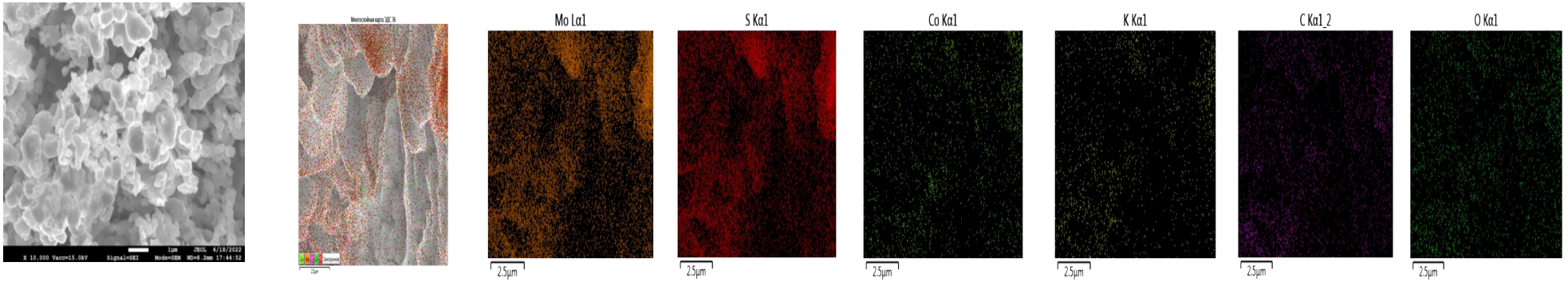
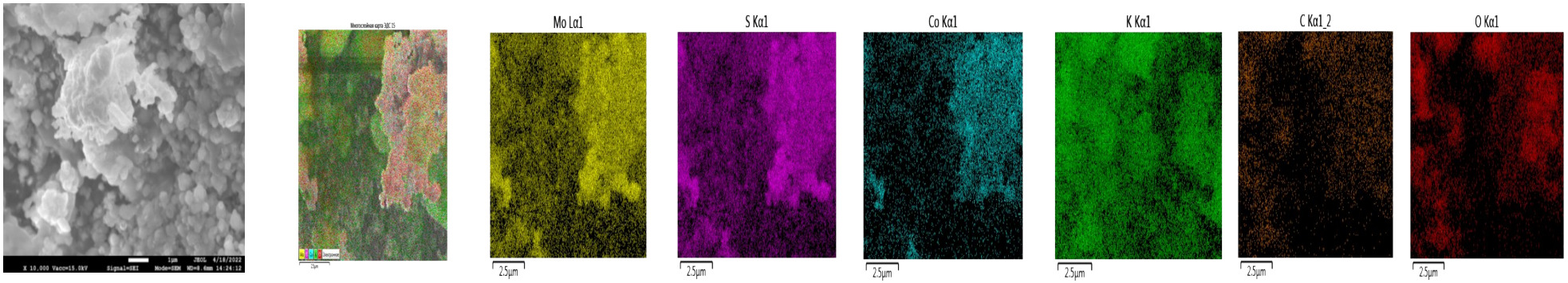


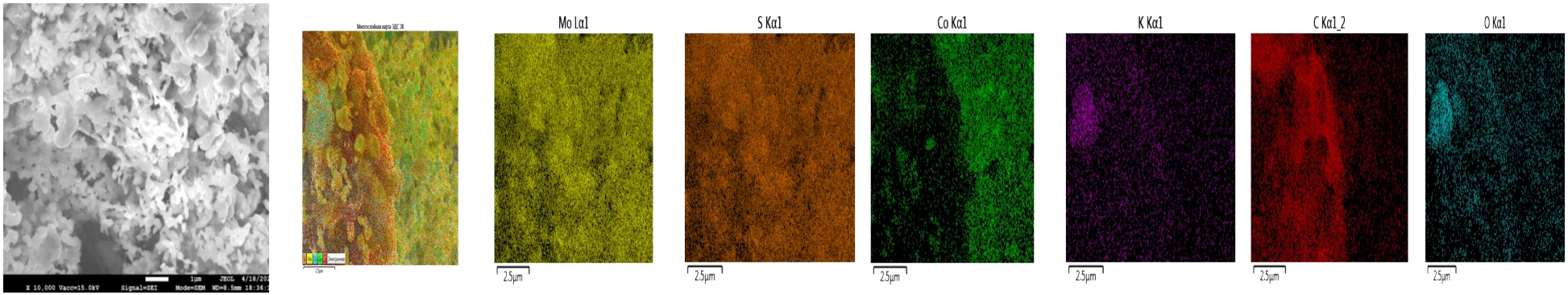
Figure S4. Additional SEM image of KCMS-org.CVD



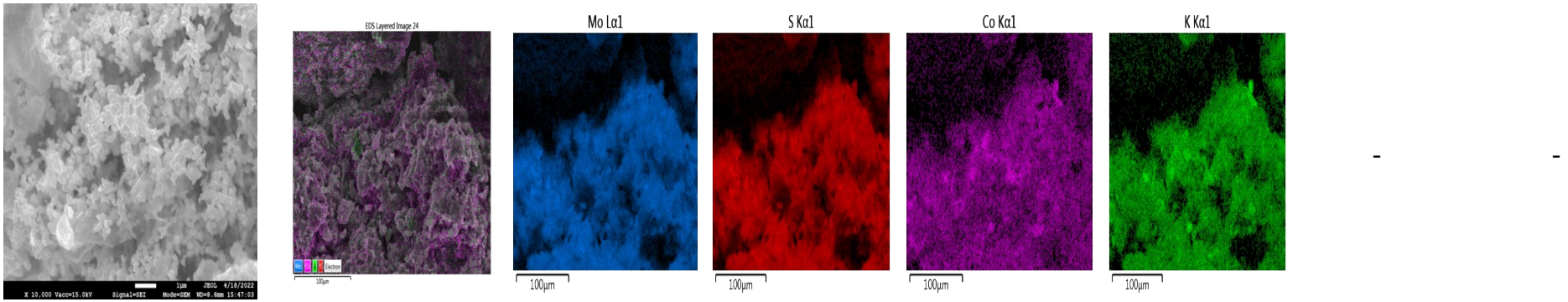
a) KCMS-Inorg.CVD



b) KCMS-org.CVD

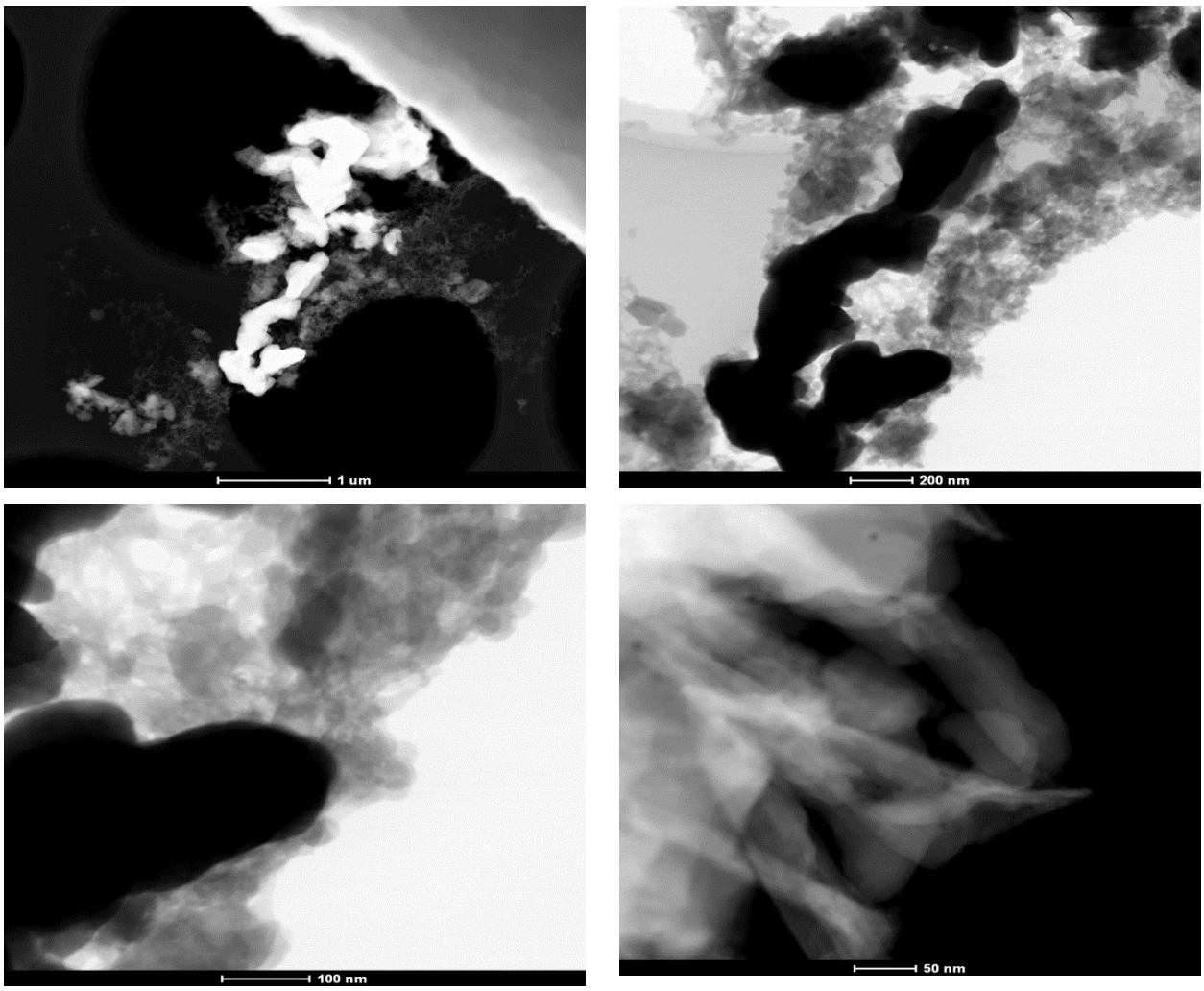


c) KCMS-Inorg.H_2S

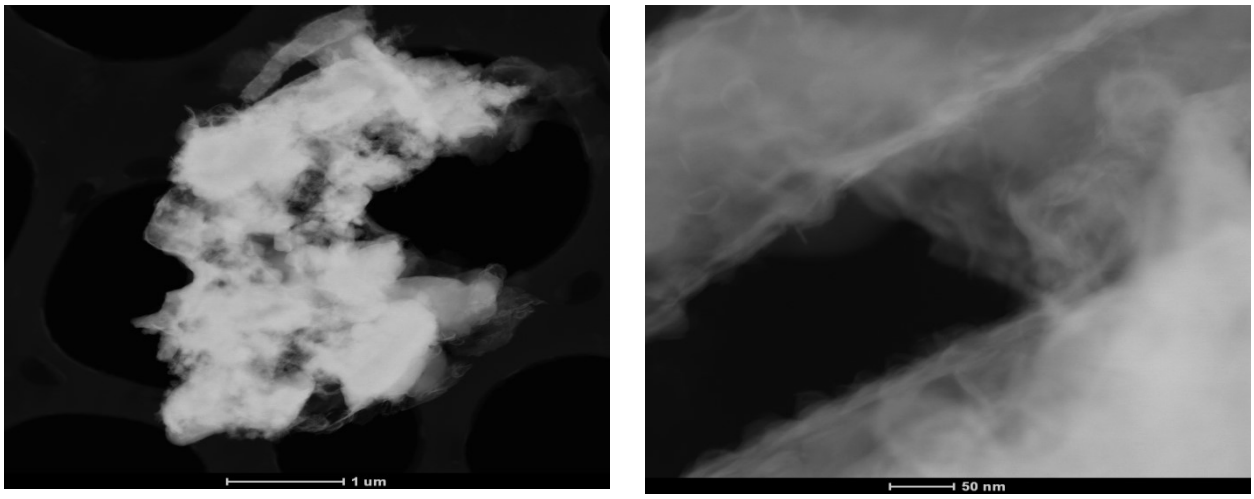


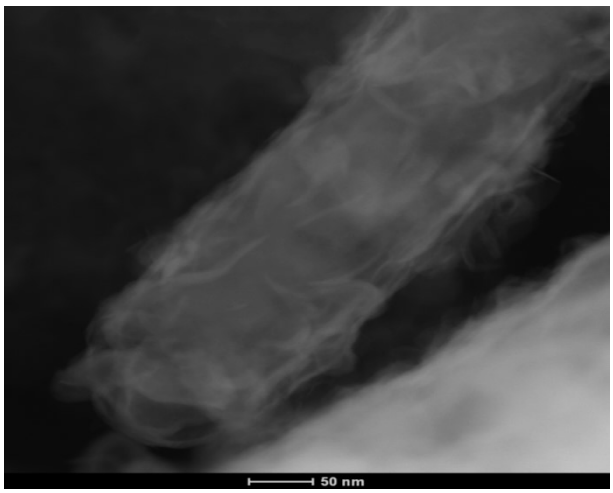
d) KCMS-org.H_2S

Figure S5. SEM/EDX of sulfided catalysts under study

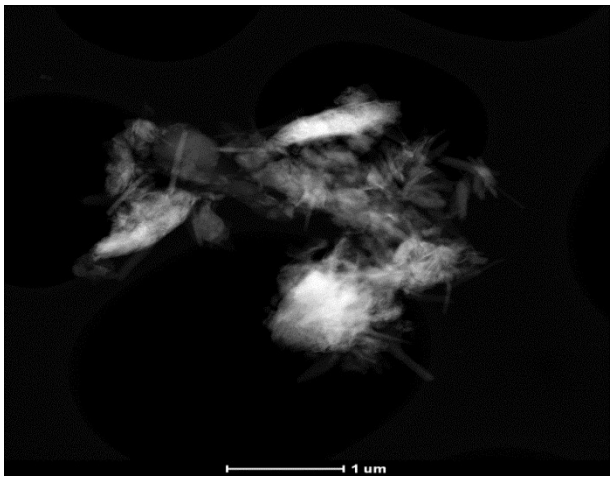


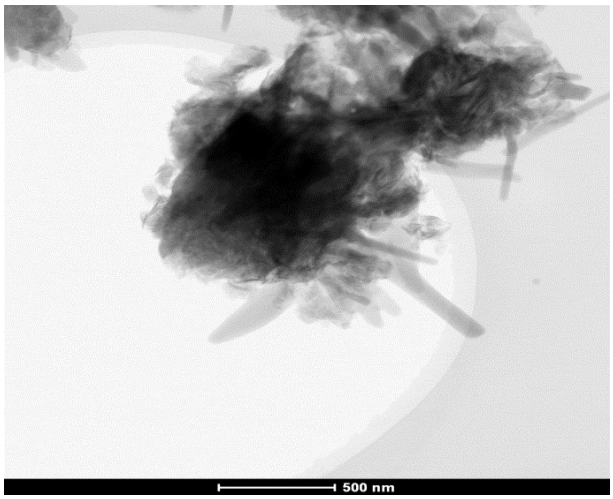
a) KCMS-Inorg.CVD

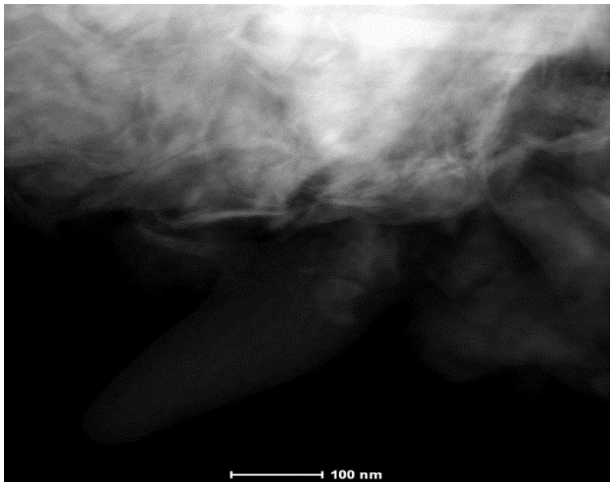


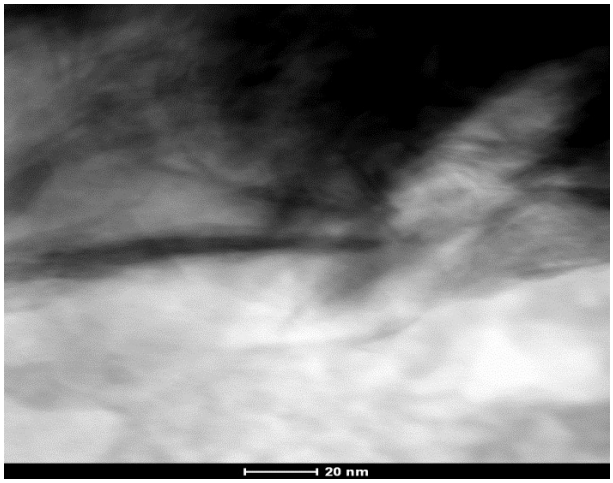


b) KCMS-Inorg.H_2S









d) KCMS-org.H_2S

Figure S5. STEM-HAADF images of the catalysts understudy in low and high magnifications

Table S1. Product distribution selectivity (with CO_2) over the catalysts understudy. Reaction conditions: T = 360 °C, P = 5 MPa, GHSV= 760 ml $(g_{cat}\ h)^{-1}$), syngas ratio (CO/H_2 =1:1)

	Selectivity (with CO_2), %			
Product	KCMS-org.CVD	KCMS-org.H_2S	KCMS-Inorg.H_2S	KCMS-Inorg.CVD
CO_2	61	18	21	13
C1	0	5	1	2
C2	2	3	8	1
C3	4	0	5	0
C4	5	0	2	1
MeOH	7	12	32	10
PrOH-2	0	0	0	0
EtOH	14	29	19	71
BuOH-2	0	0	0	0
PrOH-1	2	19	5	1
i-BuOH	4	5	6	0
BuOH-1	0	6	1	0
i-AmOH	0	2	0	0
AmOH-1	0	2	0	0

In terms of morphological evaluation, a comprehensive analysis of the slab structure can be achieved provided there is adequate contrast, which is often attainable with model catalysts like metal sulfides supported on carbon substrates [1–2]. *Baubet et al.* [3] conducted an in-depth investigation into the size and shape of alumina-supported Co-Mo sulfide structures. However, their study utilized catalysts with low metal loading and relatively high sulfidation temperatures (reaching up to 800°C), resulting in the formation of larger, well-separated slab structures (up to 10 nm) that were easier to characterize. The catalysts synthesized in our study via chemical vapor deposition (CVD) exhibit a Mo loading similar to those reported by Baubet et al. [3], but they display significantly larger visible particles. When compared to CVD-prepared catalysts, those synthesized using H_2S exhibit fewer distinct CoSx crystals or Co-rich particles. In the case of the H2S preparation method, the absence of organic additives in catalysts derived from inorganic precursors (KCMS-Inorg.H2S) may enhance the interaction between the active metals and the support. This stronger interaction reduces the extent of sulfidation and contributes to the formation of smaller MoS_2 structures [4]. Additionally, it is important to note that indistinct projections of MoS_2 crystallites are often attributed to the reoxidation of MoS2 [5–6].

References

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