

Supporting Information

Direct Synthesis of Higher Alcohols from Syngas over Modified Mo₂C Catalysts under Mild Reaction Conditions

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Table S1 The element content of various catalysts determined by ICP-OES.

Samples	Content (wt%)		
	Rh	K	Mo
Mo ₂ C	-	-	74.5
Rh/Mo ₂ C	1.8	-	73.5
RhK/Mo ₂ C	1.6	4.8	70.3
K/Mo ₂ C	-	5.2	71.4

Table S2 The catalytic performances for syngas conversion over Rh/AC and RhK/AC catalysts.

Catalysts	CO	CO ₂	Selectivity (C%, free of CO ₂)				
	Conversion %	Selectivity	CH ₃ OH	C ₂₊ Oxy	Olefins	CH ₄	C ₂₊ Alkane
Rh/AC	1.3	11.8	10.5	20.2	5.0	45.0	19.3
RhK/AC	4.5	25.0	74.1	5.0	2.2	14.9	3.8

Reaction conditions: 290 °C, H₂/CO = 1, 3 MPa, GHSV = 1200 mL·g⁻¹·h⁻¹.

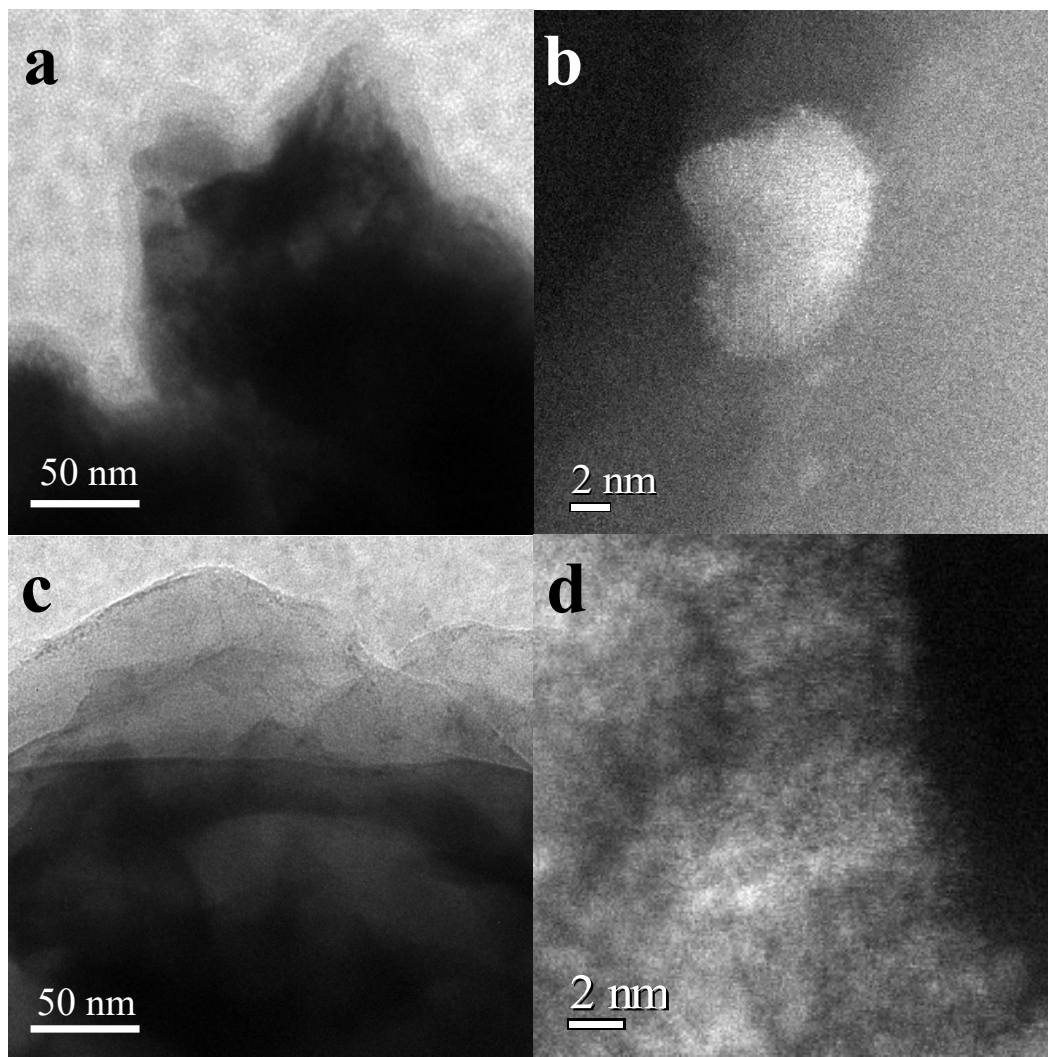


Figure S1 TEM and HAADF-STEM images of the reduced catalysts. (a, b) Rh/Mo₂C, (c, d) RhK/Mo₂C.

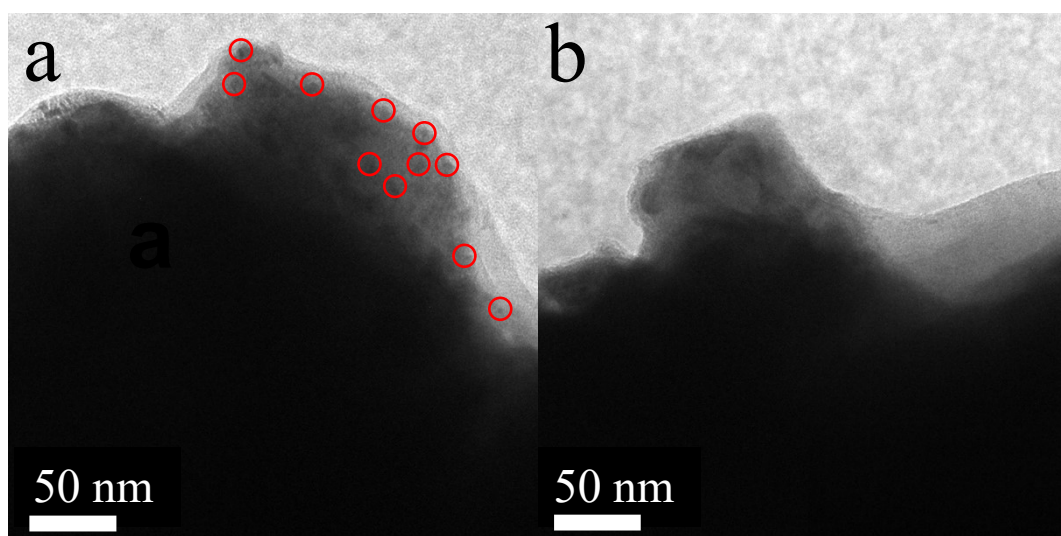


Figure S2 TEM images of the spent catalysts. (a) Rh/Mo₂C, (b) RhK/Mo₂C.

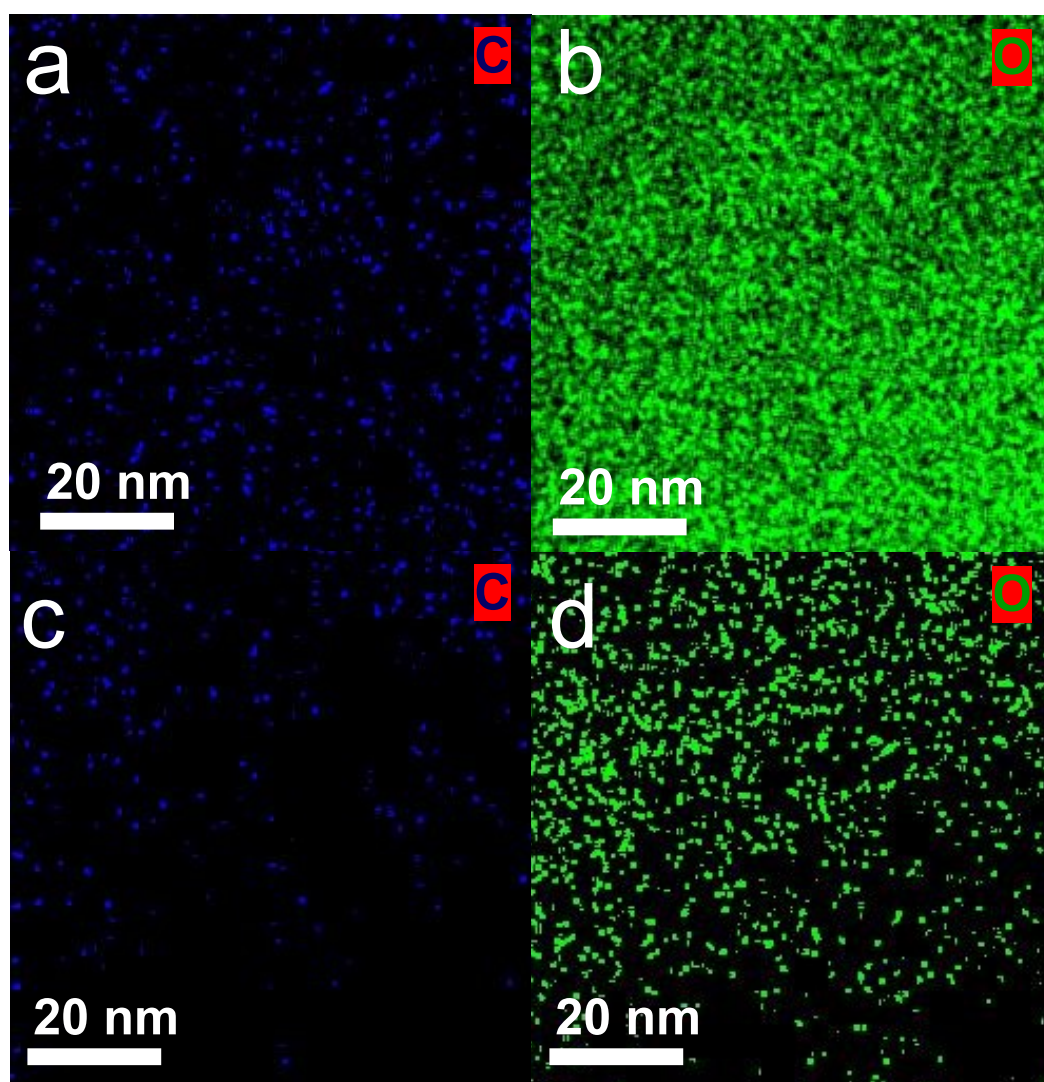


Figure S3 Elemental mapping of C and O for spent Rh/Mo₂C (a, b) and

RhK/Mo₂C (c, d) catalysts.

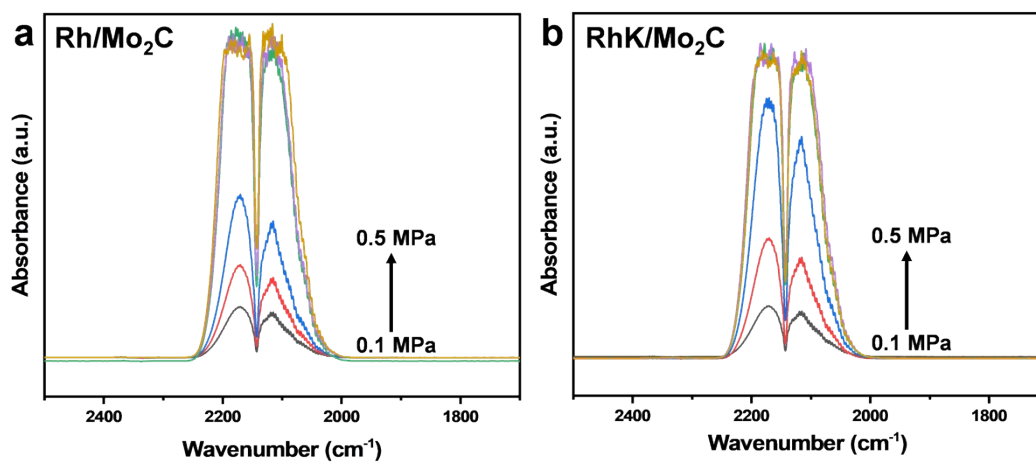


Figure S4 In situ DRIFTs of CO adsorption from 0.1 to 0.5 MPa at 50 °C over Rh/Mo₂C (a) and RhK/Mo₂C (b) catalysts.

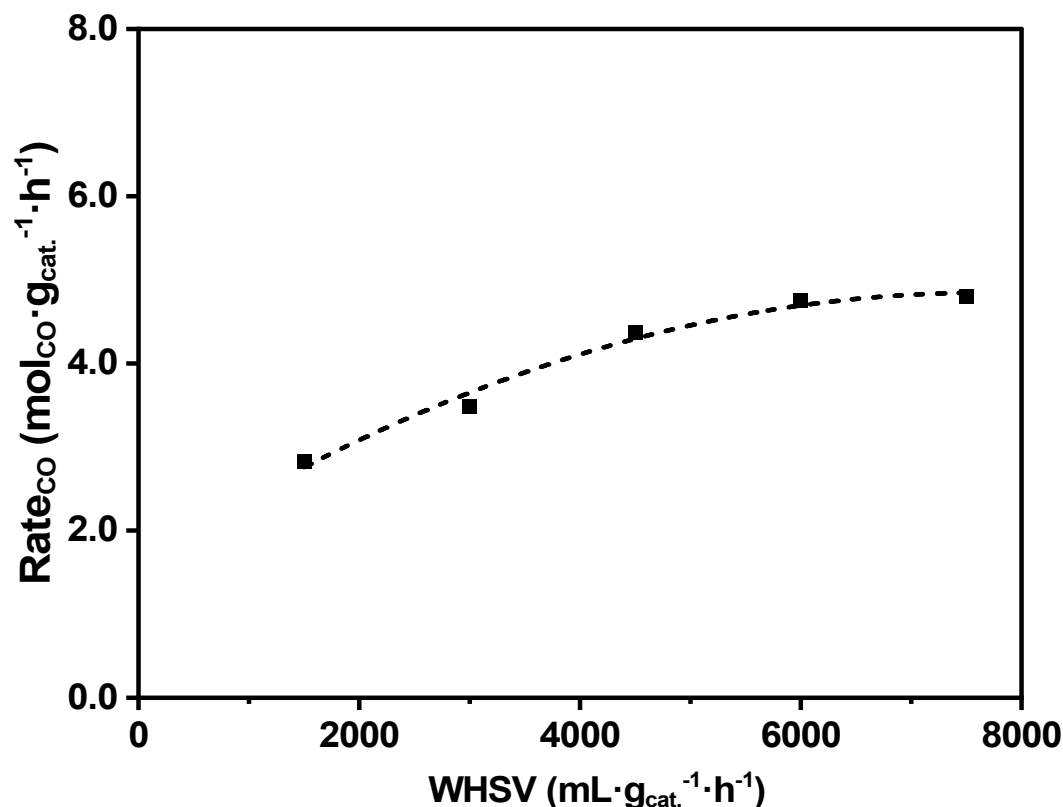


Figure S5 Dependence of CO consumption rate on WHSV.

(Conditions: H₂/CO=1, 290 °C, 1 MPa, 0.4 g of catalyst diluted with 2 g quartz)

For kinetic study, the diffusion effects were excluded by adjusting the WHSV over RhK/Mo₂C catalyst. With the increase of WHSV from 1500 to 7500 mL · g_{cat.}⁻¹ · h⁻¹ (Figure S5), CO consumption rate increased and then remained almost constant when WHSV reached 6000 mL · g_{cat.}⁻¹ · h⁻¹, demonstrating a negligible effect on mass-transfer diffusion when WHSV was higher than 6000 mL · g_{cat.}⁻¹ · h⁻¹. In the kinetic study, WHSV of 7500 mL · g_{cat.}⁻¹ · h⁻¹ was used to avoid the effect of mass transfer. In addition, to exclude the effect of heat transfer, 0.4 g of catalyst was diluted with 2 g quartz sand to remove the reaction heat.

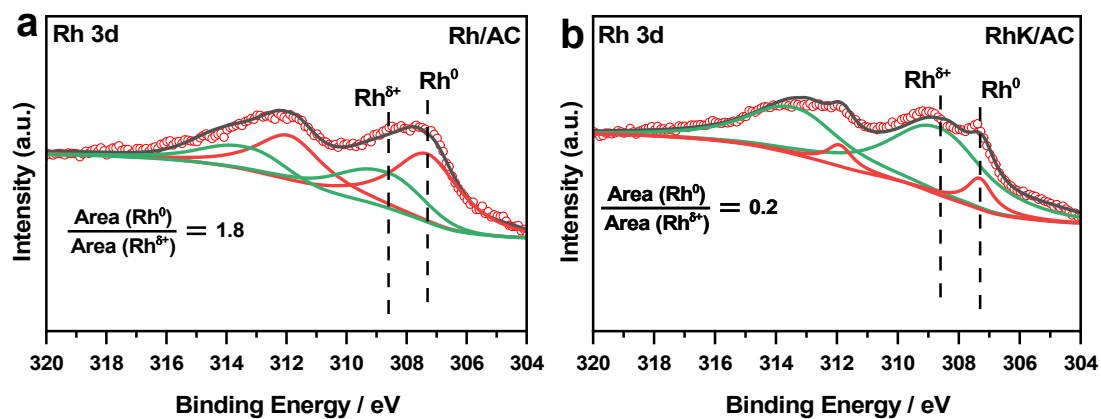


Figure S6 Rh 3d XPS spectra of (a) Rh/AC, (b) RhK/AC after reduction in syngas flow.

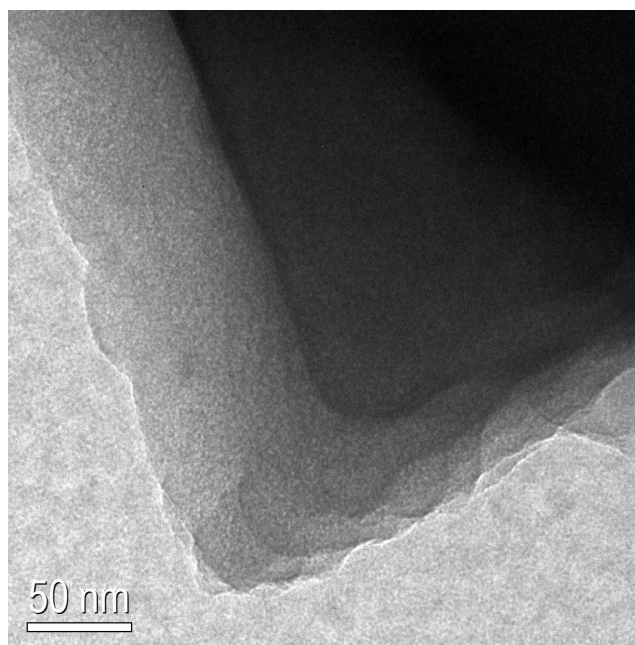


Figure S7. TEM image of the spent RhK/AC catalyst.

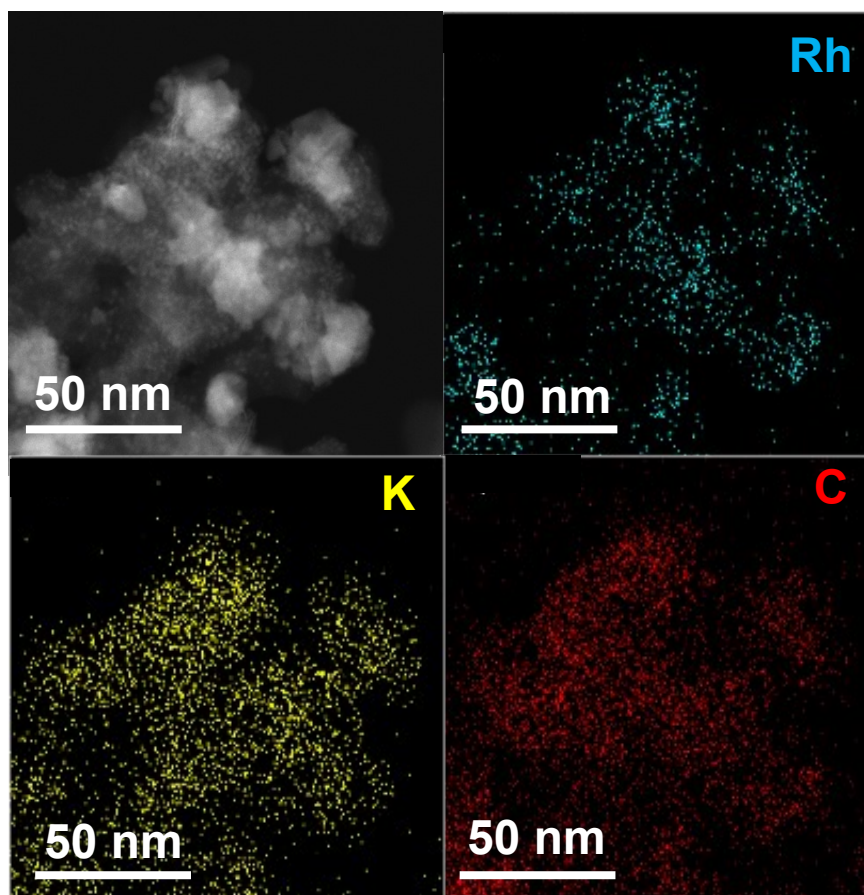


Figure S8. HAADF-STEM image and the corresponding EDS elemental mapping images of the spent RhK/AC catalyst.

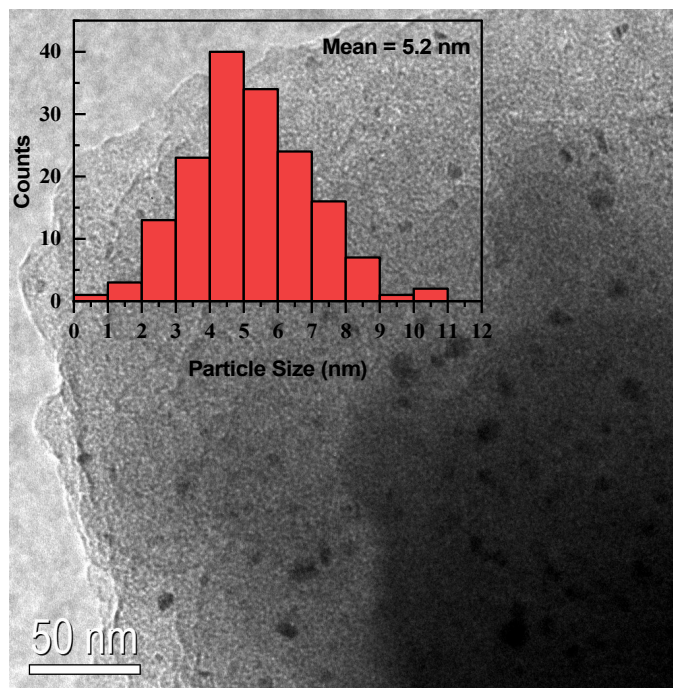


Figure S9. TEM image of the spent Rh/AC catalyst with size distribution of Rh nanoparticles.