Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information

Synthesis of higher alcohols by CO hydrogenation on a K-promoted Ni–Mo catalyst derived from Ni–Mo phyllosilicate

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Table S1

XPS profile and relative content (molar fraction) of Ni^{n+} species at the surface of reduced catalysts.

Catalyst	Relative content (mol%)		
	Ni^0-$2p_{3/2}$ ≈ 852.6 eV (B. E.)	NiO-$2p_{3/2}$ ≈ 854.4 eV (B. E.)	NiO(OH)-$2p_{3/2}$ ≈ 856.2 eV (B. E.)
$K_{0.5}$-($Ni_1Mo_{0.25}$)Si-PS	20.8	34.3	44.9
$K_{0.5}Mo_{0.25}$/NiSi-PS	30.6	35.9	33.5
$K_{0.5}$-($Ni_1Mo_{0.25}$)Si-DP	44.2	30.7	25.1

Table S2

XPS profile and relative content (molar fraction) of the Mo^{n+} species at the surface of reduced catalysts.

Catalyst	B. E. of Mo($3d_{5/2}$) (eV)				Relative contents (mol%)			
	Mo^0	Mo^{3+}	Mo^{4+}	Mo^{6+}	Mo^0	Mo^{3+}	Mo^{4+}	Mo^{6+}
$K_{0.5}$-($Ni_1Mo_{0.25}$)-PS	228.2	229.8	230.9	232.2	23.8	32.1	27.9	16.2
$K_{0.5}Mo_{0.25}$/NiSi-PS	228.6	229.8	230.9	232.8	25.8	15.8	26.7	31.7
$K_{0.5}$-($Ni_1Mo_{0.25}$)-DP	228.3	229.8	230.9	232.6	52.2	15.2	17.7	14.9

Table S3

Catalytic activity of $K_{0.5}$-(Ni_1Mo_x)Si-PS for synthesis of HAs from syngas.

Catalyst	X(CO) (%)	Selectivity (%)			Alcohol distribution (%)		STY_{ROH} (mg/(g·h))
		HCs	ROH	CO_2	MeOH	C_{2+}-OH	
$K_{0.5}$-($Ni_1Mo_{0.15}$)Si-PS	5.5	29.5	32.8	37.7	40.3	59.7	55.9
$K_{0.5}$-($Ni_1Mo_{0.25}$)Si-PS	6.6	25.2	43.7	31.1	34.6	65.4	76.4
$K_{0.5}$-($Ni_1Mo_{0.35}$)Si-PS	2.0	45.2	34.1	20.7	49.0	51.0	14.0

Reaction conditions: P = 3.0 MPa, GHSV = 3000 mL/(g·h), n(H_2)/n(CO) = 1, T = 240 °C.

Table S4

Catalytic activity of catalysts prepared by different methods for synthesis of HAs from syngas.

Catalyst	Ni/Mo/K molar ratio[c]	X(CO) (%)	Selectivity (%)			Alcohol distribution (%)		STY_{ROH} (mg/(g·h))
			HCs	ROH	CO_2	MeOH	C_{2+}-OH	
$K_{0.5}$-($Ni_1Mo_{0.25}$)Si-PS[a]	1.00/0.11/0.34	6.6	25.1	43.8	31.1	34.6	65.4	76.4
$K_{0.5}Mo_{0.25}$/Ni_1Si-PS[a]	1.00/0.13/0.43	3.6	20.1	42.4	37.5	46.9	53.1	46.9
$K_{0.5}$-($Ni_1Mo_{0.25}$)Si-DP[a]	1.00/0.18/0.60	0	0	0	0	0	0	0
$K_{0.5}$-($Ni_1Mo_{0.25}$)Si-DP[b]	1.00/0.18/0.60	5.8	27.4	37.9	34.7	43.6	56.4	43.5

Reaction conditions: P = 3.0 MPa, GHSV = 3000 mL/(g·h), n(H_2)/n(CO) = 1, [a] T = 240 °C, [b] T = 300 °C. [c] The data were estimated by XPS.

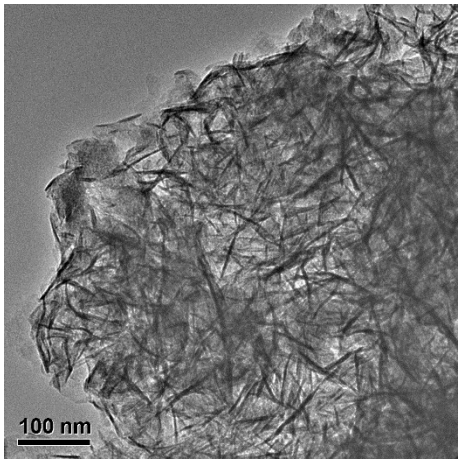

Fig. S1 TEM image of as-calcined K_0-($Ni_1Mo_{0.25}$)Si-PS.

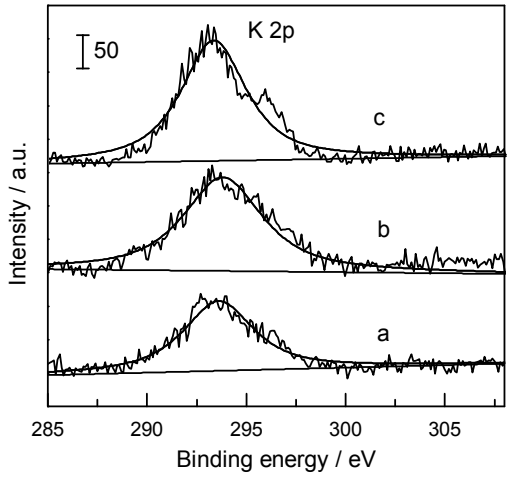

Fig. S2 K 2p XPS profiles of the as-reduced catalyst of (a) $K_{0.5}$-($Ni_1Mo_{0.25}$)Si-PS, (b) $K_{0.5}Mo_{0.25}$/Ni_1Si-PS, and (c) $K_{0.5}$-($Ni_1Mo_{0.25}$)Si-DP.

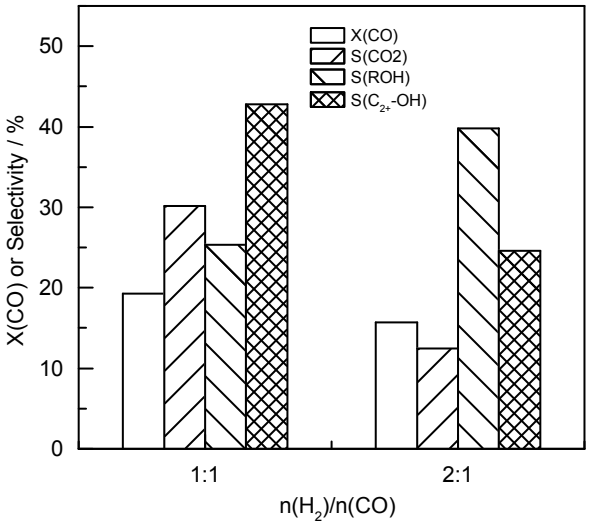

Fig. S3 Influence of H_2/CO molar ratio on the performance of $K_{0.1}$-($Ni_1Mo_{0.25}$)Si-PS. Reaction conditions: T = 220 ºC, P = 2.0 MPa, GHSV = 3000 mL/(g·h).

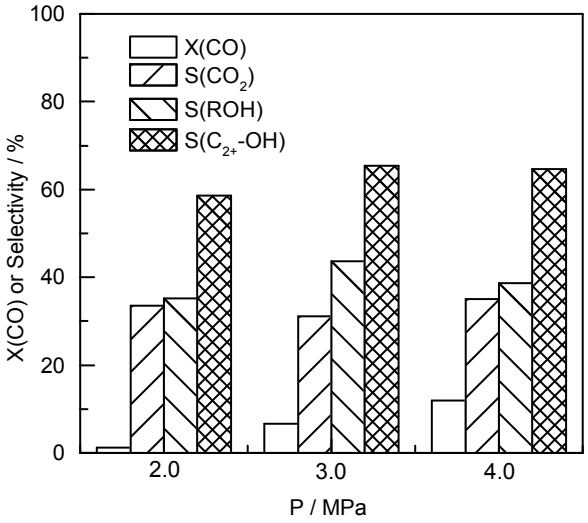

Fig. S4 Influence of pressure on the performance of $K_{0.5}$-($Ni_1Mo_{0.25}$)Si-PS. Reaction conditions: *T* = 240 ºC, *P* = 3.0 MPa, GHSV = 3000 mL/(g·h), n(H_2)/n(CO) = 1.

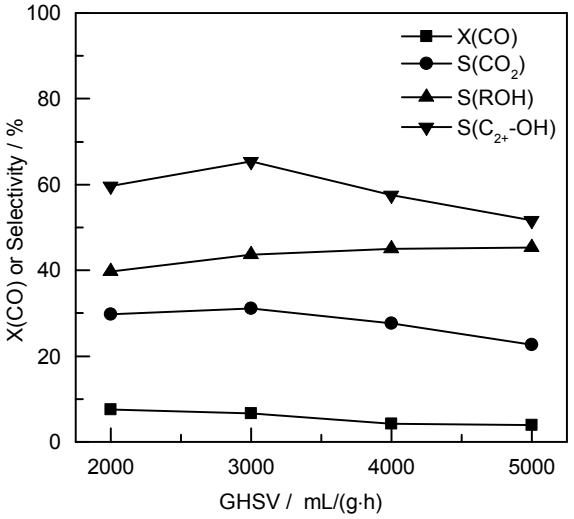

Fig. S5 Influence of GHSV on the performance of $K_{0.5}$-($Ni_1Mo_{0.25}$)Si-PS. Reaction conditions: *T* = 240 ºC, *P* = 3.0 MPa, GHSV = 3000 mL/(g·h), n(H_2)/n(CO) = 1.

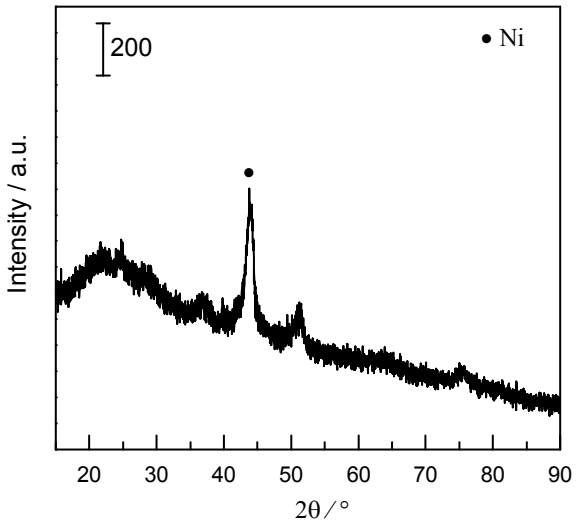

Fig. S6 XRD pattern of as-used $K_{0.5}$-($Ni_1Mo_{0.25}$)Si-DP performed for 48 h under the reaction conditions of P = 3.0 MPa, T= 240 °C, GHSV = 3000 mL/(g·h), $n(H_2)/n(CO)$ = 1.

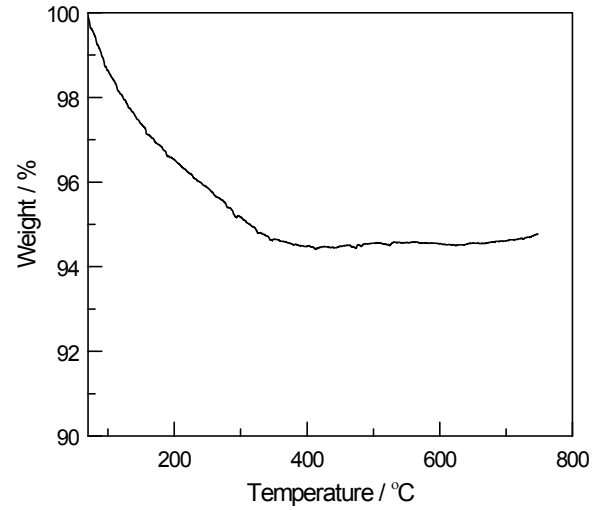

Fig. S7 TG curve of as-used $K_{0.5}$-($Ni_1Mo_{0.25}$)Si-DP performed for 48 h under the reaction conditions of P = 3.0 MPa, T = 240 °C, GHSV = 3000 mL/(g·h), $n(H_2)/n(CO)$ = 1.