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Effects of Graphitization of Carbon Nanosphere on Hydrodeoxygenation Activity of Molybdenum Carbide

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Table S1 XPS results for the C 1s spectra of different carbon materials.

Supports	Atomic percentage (%)			
	C-C in plane	C-C defects	C-O	C=O
CNS	26.6	32.2	17.7	23.5
GCNS-1	37.6	31.2	14.3	16.9
GCNS-10	55.3	19.4	10.9	14.4
GCNS-50	65.9	13.8	8.7	11.6
MWNT	70.3	5.6	13.5	10.6
AC	22.0	25.7	31.6	20.7

Table S2 XPS results of the Mo 3d spectra of different catalysts.

Catalysts	Temperature (K)	Binding energy (eV) (Atomic percentage (%))				
		Mo^{2+}	$Mo^{2\sim4+}$	Mo^{4+}	$Mo^{4\sim6+}$	Mo^{6+}
20%Mo_2C/CNS	393 [a]	228.21 (10.9)	228.70 (4.4)	229.41 (23.8)	231.18 (20.9)	232.53 (40.0)
	533	228.20 (36.7)	228.72 (11.4)	229.38 (25.4)	231.20 (17.3)	232.49 (9.3)
	573	228.18 (52.3)	228.69 (11.3)	229.39 (15.8)	231.20 (18.9)	232.50 (1.6)
20%Mo_2C/GCNS-1	393 [a]	228.33 (12.7)	228.68 (18.6)	229.30 (21.6)	231.19 (8.6)	232.42 (38.5)
	533	228.30 (48.2)	228.71 (12.0)	229.28 (17.1)	231.21 (11.6)	232.37 (11.1)
	573	228.28 (56.3)	228.70 (24.9)	229.32 (14.3)	231.17 (2.0)	232.39 (2.5)
20%Mo_2C/GCNS-10	393 [a]	228.39 (21.8)	228.71 (14.7)	229.27 (22.1)	231.22 (17.6)	232.38 (23.9)
	533	228.38 (60.9)	228.68 (8.3)	229.30 (19.3)	231.19 (4.0)	232.43 (7.5)
	573	228.36 (67.7)	228.68 (12.3)	229.28 (11.4)	231.23 (5.4)	232.38 (3.1)
20%Mo_2C/GCNS-50	393 [a]	228.37 (21.3)	228.71 (13.3)	229.41 (28.3)	231.17 (8.7)	232.36 (28.5)
	533	228.39 (61.1)	228.69 (14.8)	229.40 (11.2)	231.21 (6.8)	232.42 (6.1)
	573	228.40 (74.0)	228.69 (17.2)	229.38 (5.0)	231.22 (2.5)	232.40 (1.4)
20%Mo_2C/MWNT	393 [a]	228.41 (21.7)	228.68 (15.0)	229.32 (25.7)	231.20 (20.9)	232.51 (16.7)
	533	228.41 (63.7)	228.70 (7.6)	229.28 (19.9)	231.18 (3.8)	232.48 (4.9)
	573	228.40 (75.5)	228.71 (11.3)	229.30 (8.3)	231.20 (3.7)	232.50 (1.2)
20%Mo_2C/AC	393 [a]	228.21 (3.8)	228.72 (11.7)	229.37 (24.1)	231.18 (10.9)	232.53 (49.5)
	533	228.16 (35.4)	228.69 (8.3)	229.41 (5.7)	231.22 (35.5)	232.49 (15.2)
	573	228.18 (48.1)	228.70 (12.0)	229.39 (5.5)	231.21 (26.6)	232.51 (7.9)

[a] 393K is the temperature at which the samples were pretreated in Ar.

Table S3 XPS results of the C 1s spectra of different catalysts.

Catalysts	Temperature (K)	Binding energy (eV) (Atomic percentage (%))				
		C-Mo	C-C in plane	C-C defects	C-O	C=O
20%Mo_2C/CNS	393 [a]	284.21 (7.9)	284.58 (31.8)	285.51 (33.6)	286.71 (12.1)	288.67 (14.6)
	533	284.20 (11.6)	284.61 (32.1)	285.49 (33.7)	286.71 (8.9)	288.67 (13.7)
	573	284.20 (16.6)	284.60 (32.2)	285.51 (33.9)	286.70 (6.4)	288.69 (10.9)
20%Mo_2C/GCNS-1	393 [a]	284.16 (10.0)	284.58 (41.7)	285.50 (28.2)	286.68 (11.2)	288.68(8.9)
	533	284.15 (14.6)	284.61 (41.3)	285.47 (28.2)	286.70 (7.5)	288.69 (8.4)
	573	284.15 (18.0)	284.61 (41.9)	285.51 (28.3)	286.67 (3.8)	288.67 (8.0)
20%Mo_2C/GCNS-10	393 [a]	284.13 (11.1)	284.60 (54.0)	285.51 (17.5)	286.71 (9.5)	288.65 (7.9)
	533	284.14 (15.9)	284.59 (54.4)	285.50 (17.4)	286.69 (3.4)	288.66 (8.9)
	573	284.14 (18.6)	284.59 (54.5)	285.50 (17.3)	286.69 (2.1)	288.70 (7.5)
20%Mo_2C/GCNS-50	393 [a]	283.98 (9.5)	284.60 (63.5)	285.47 (14.9)	286.69 (7.8)	288.69 (4.3)
	533	284.00 (15.5)	284.58 (63.1)	285.50 (14.8)	286.71 (2.7)	288.70 (3.9)
	573	284.01 (18.7)	284.60 (63.1)	285.48 (15.0)	286.68 (1.1)	288.72 (2.1)
20%Mo_2C/MWNT	393 [a]	284.00 (10.8)	284.58 (65.4)	285.51 (8.4)	286.70 (8.1)	288.72 (7.3)
	533	283.98 (16.6)	284.58 (65.4)	285.48 (8.7)	286.68 (3.2)	288.70 (6.1)
	573	284.01 (19.1)	284.60 (65.4)	285.50 (8.2)	286.68 (2.1)	288.69 (5.2)
20%Mo_2C/AC	393 [a]	284.18 (8.5)	284.62 (28.1)	285.47 (27.6)	286.71 (24.3)	288.67 (11.5)
	533	284.17 (12.7)	284.60 (28.3)	285.50 (27.8)	286.69 (21.8)	288.69 (9.4)
	573	284.20 (17.5)	284.62 (28.5)	285.48 (28.0)	286.70 (17.1)	288.70 (8.9)

[a] 393K is the temperature at which the samples were pretreated in Ar.

Table S4 Results of the parallel reactions of 20%Mo_2C catalysts on different supports [a].

Carbon supports	Product distribution (%)								Conversion (%)	Yield (%)
	C_{15}	C_{16}	$C_{16}^{=}$	$C_{17}^{=}$	C_{17}	$C_{18}^{=}$	C_{18}	Others		
AC	0.1	8.6	0.6	0.3	0.7	15.4	32.9	8.9	67.5	58.6
CNS	0.3	9.2	0.8	0.5	1.8	9.4	44.0	8.1	74.1	66.0
GCNS-1	0.4	13.7	0.3	0.6	1.8	12.6	53.3	3.4	86.0	82.6
GCNS-10	0.2	14.7	0.56	0.2	1.7	6.4	65.	1.8	91.3	89.5
GCNS-50	0.3	14.0	0.3	0.6	2.4	6.7	57.1	3.2	84.5	81.3
MWNT	0.3	14.3	0.6	0.4	1.4	7.5	66.8	2.8	94.1	91.4

[a] Parallel experiments were conducted for reproducibility concerns, and the relative deviation of conversion and yield of hydrocarbons for each pair of parallel reactions were less than 2%.

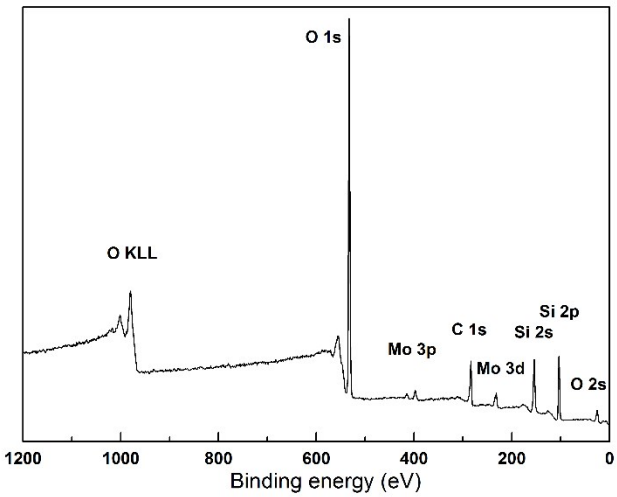

Fig. S1 XPS spectra of 20%Mo_2C/GCNS-50 at room temperature.

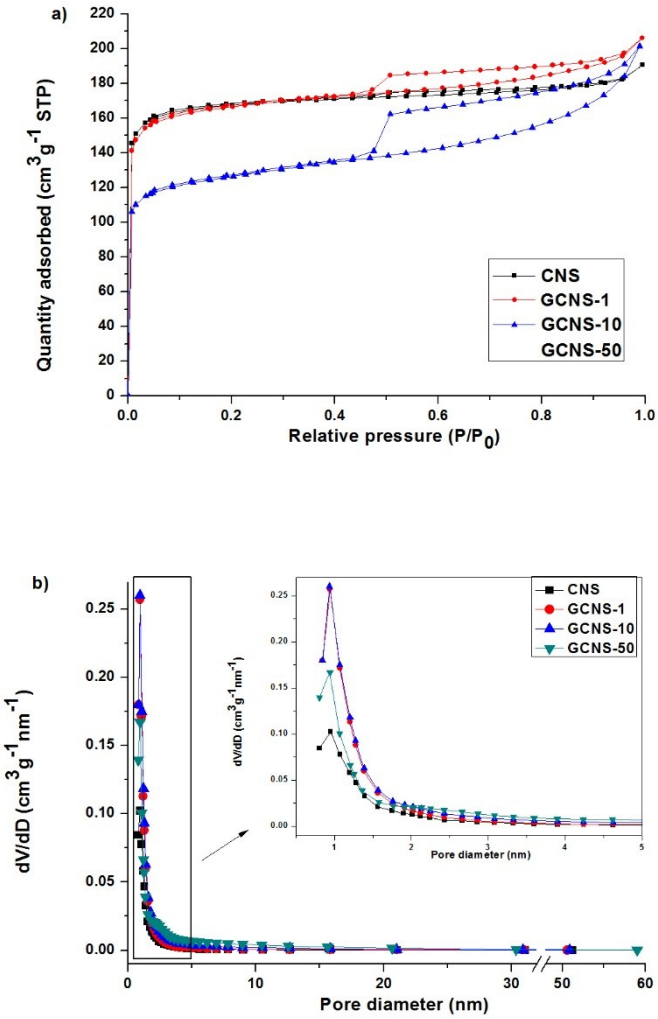

Fig. S2 N_2 adsorption-desorption isotherms (a) and pore size distributions (b) for CNS, GCNS-1, GCNS-10, and GCNS-50.

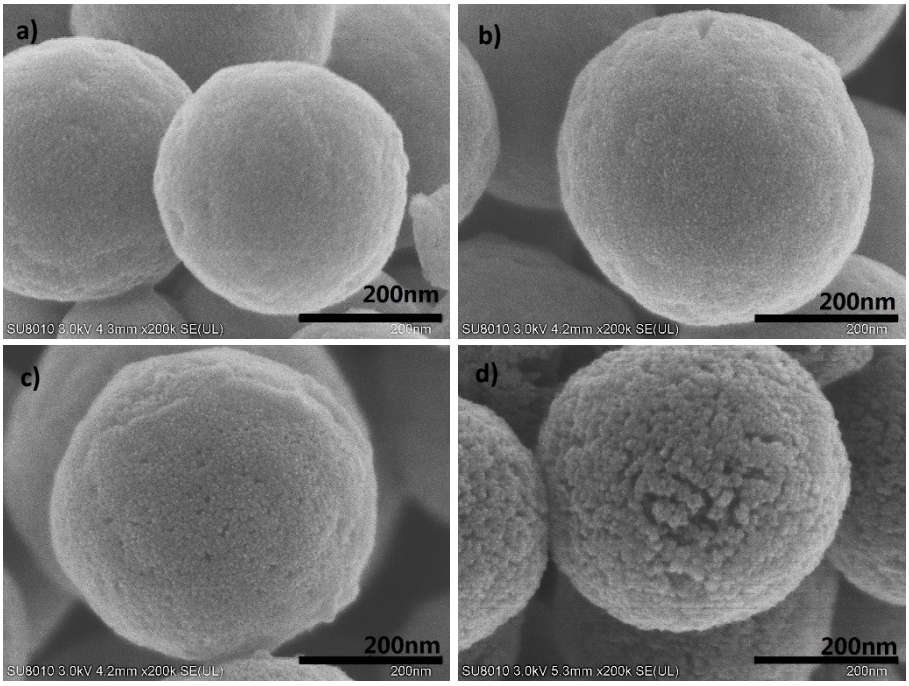

Fig. S3 SEM images of a) 5%, b) 10%, c) 20%, and d) 40%Mo_2C/CNS catalysts.

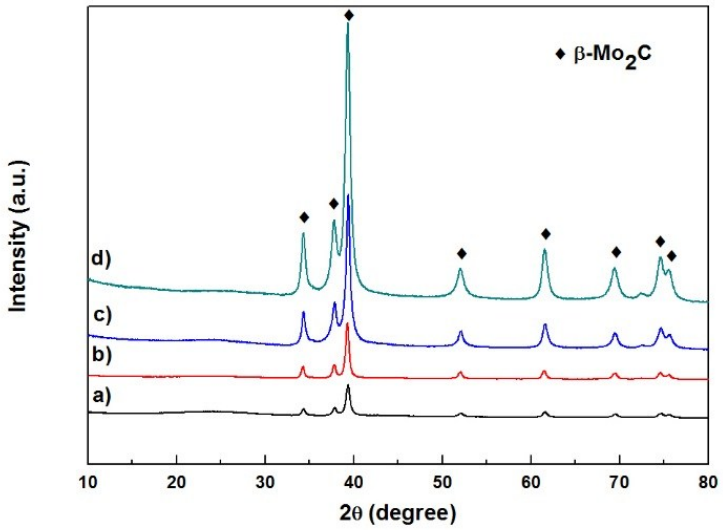

Fig. S4 XRD patterns of a) 5%, b) 10%, c) 20%, and d) 40%Mo_2C/CNS catalysts.

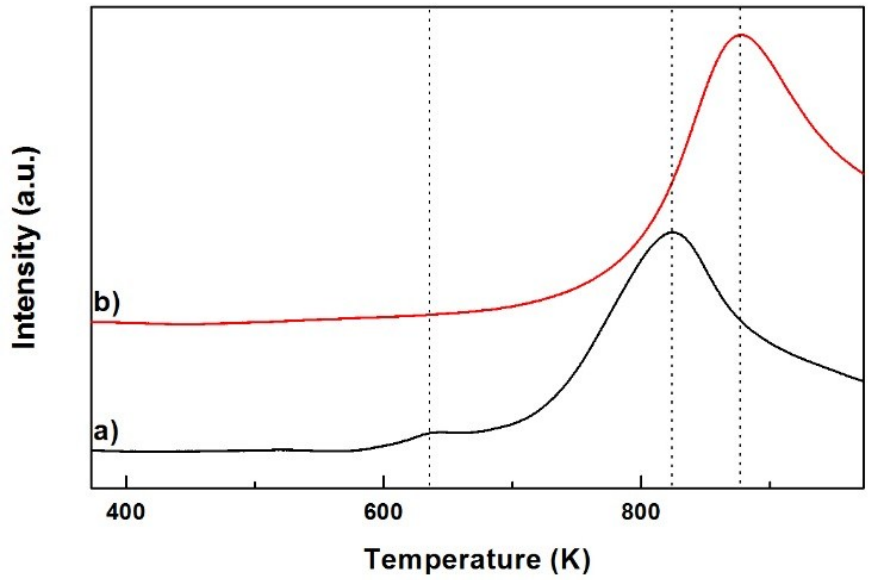

Fig. S5 H_2-TPR profiles of a) 20%Mo_2C/CNS and b) 20%Mo_2C/GCNS-10 precursors.

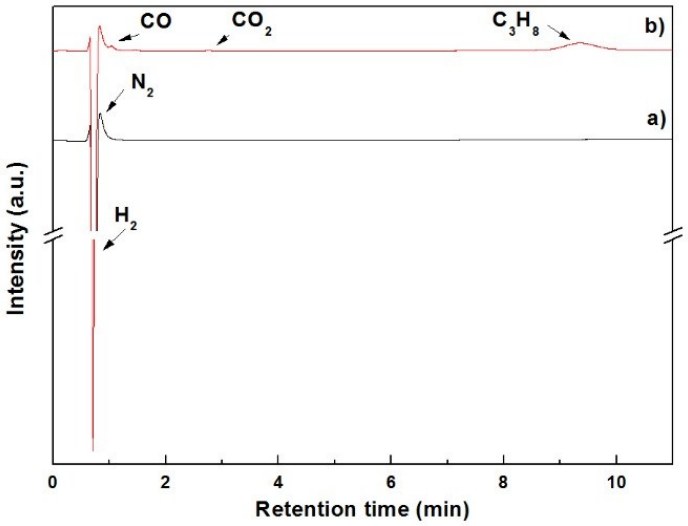

Fig. S6 Gas chromatogram of gaseous phase in the autoclave a) before reaction and b) after reaction.