catalysts

MDPI

Supporting information

Low-temperature hydrogenation of toluene using an iron-promoted molybdenum carbide catalyst

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Table S1. Textural properties and elemental compositions of the as-prepared Fe-Mo_2C catalysts with different Fe loadings.

Sample	Fe Doping[a] (at%(Fe/(Fe + Mo))		Surface Area[b] (m^2/g)
	Nominal Value	Real Value	
β-Mo_2C	N/A	N/A	6.8
1.5Fe-Mo_2C-550	1.5	1.5	8.03
5Fe- Mo_2C-550	5	5.2	5.34
10Fe- Mo_2C-550	10	10.5	11.88
15Fe- Mo_2C-550	15	15.8	15.64
20Fe- Mo_2C-550	20	20.7	25.37
20Fe- Mo_2C-600	20	20.7	17.59
20Fe- Mo_2C-650	20	20.7	9.30
20Fe- Mo_2C-700	20	20.7	8.06

[a] Determined via ICP-OES. [b] Determined via N_2 adsorption. N/A: no data.

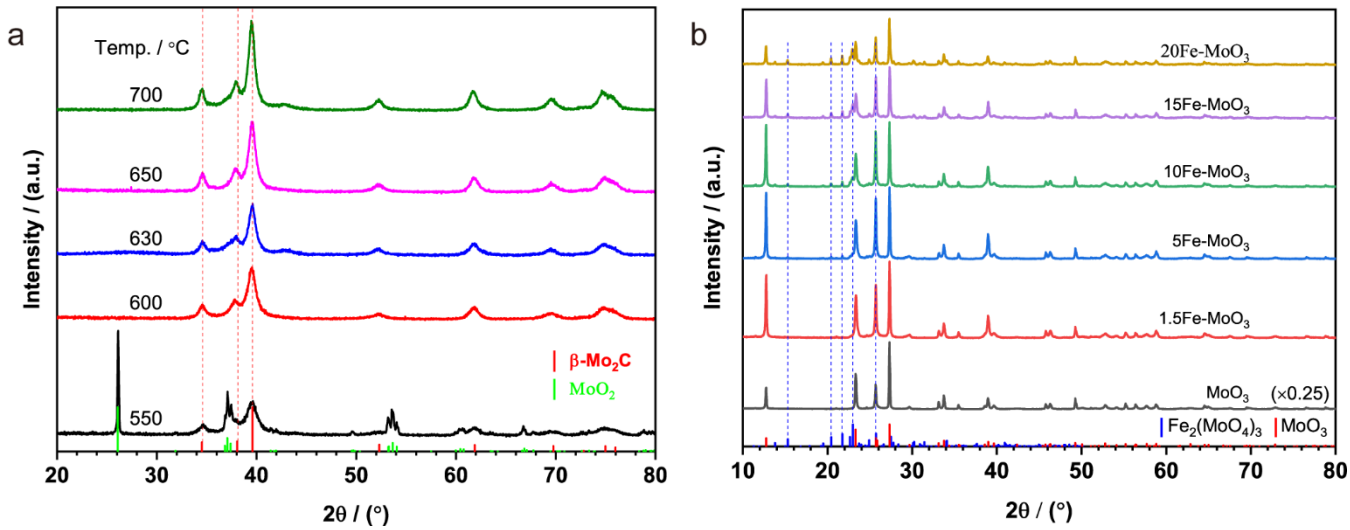

Figure S1. (a) XRD patterns of beta-Mo_2C prepared at different final temperatures (550 °C, 600 °C, 630 °C, 650 °C and 700 °C), (b) XRD patterns of Fe-MoO_3 precursors.

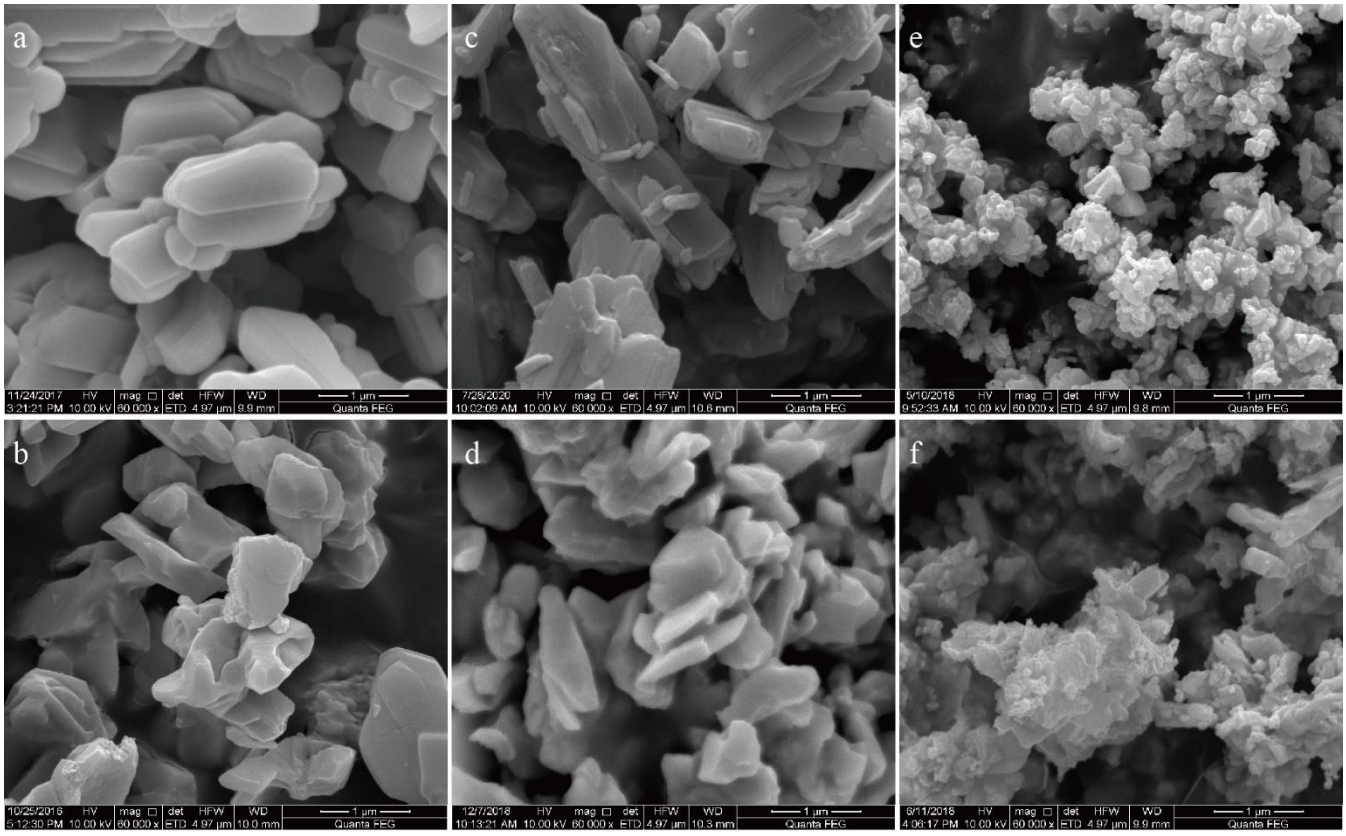

Figure S2. SEM images of (a) MoO_3, (b) beta-Mo_2C, (c) 1.5Fe-MoO_3, (d) 1.5Fe- Mo_2C-550, (e) 10Fe-MoO_3, (f) 10Fe- Mo_2C-550.

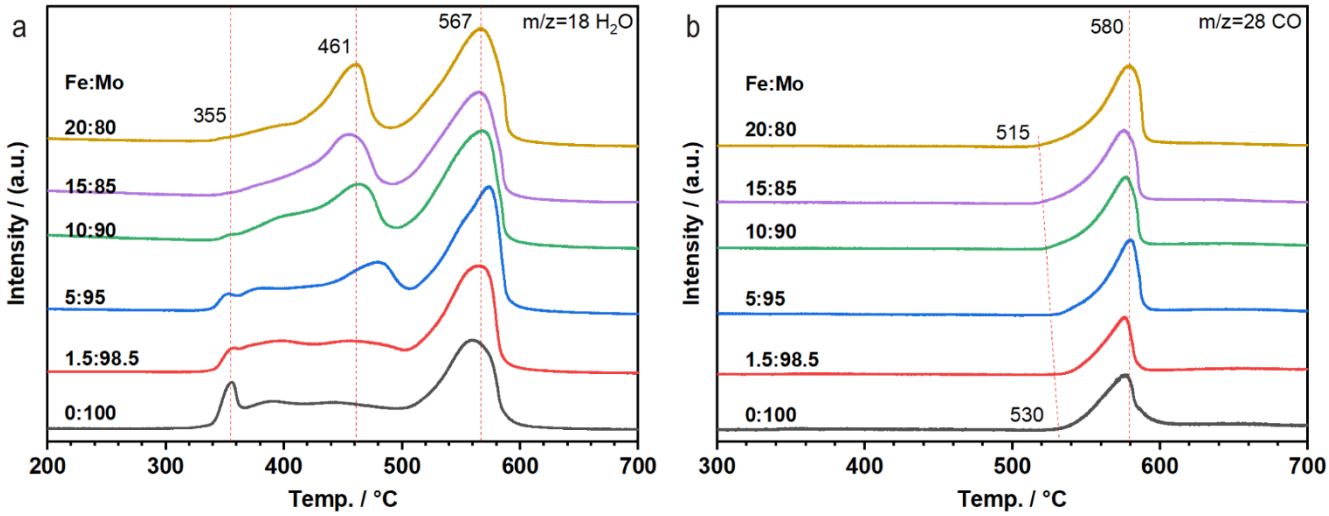

Figure S3. Temperature-programmed carburization of Fe-MoO_3 and using MS to detect the vent gas of (a) H_2O (m/z=18) and (b) CO (m/z=28).

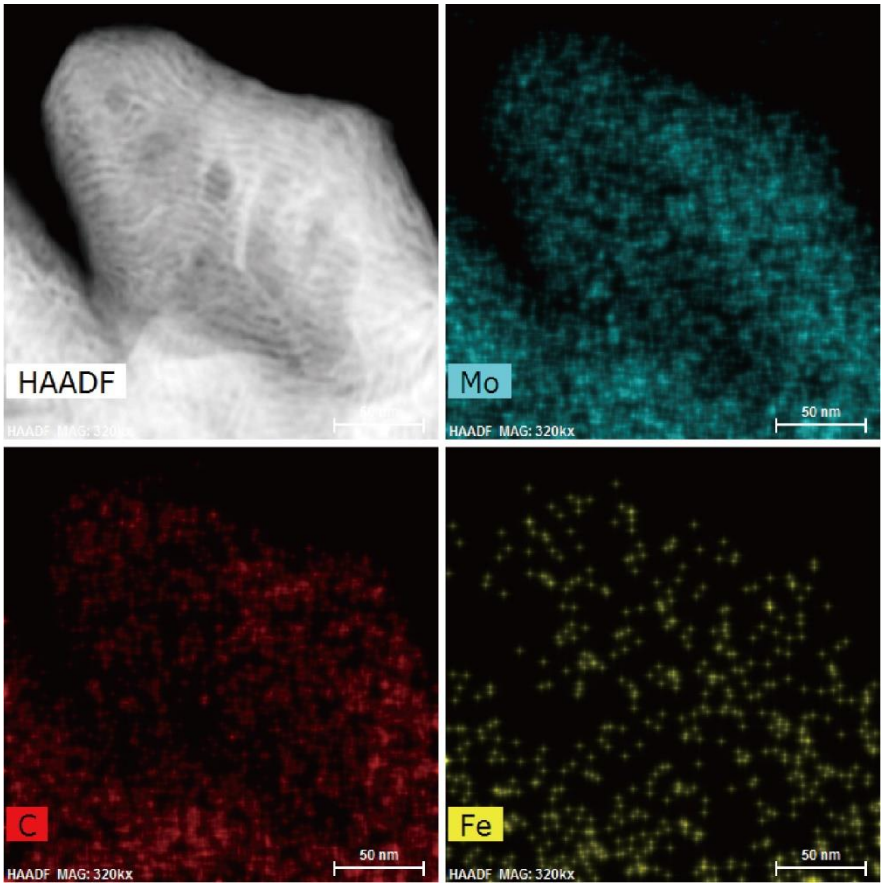

Figure S4. STEM image and corresponding element mapping picture of 1.5Fe- Mo_2C-550.

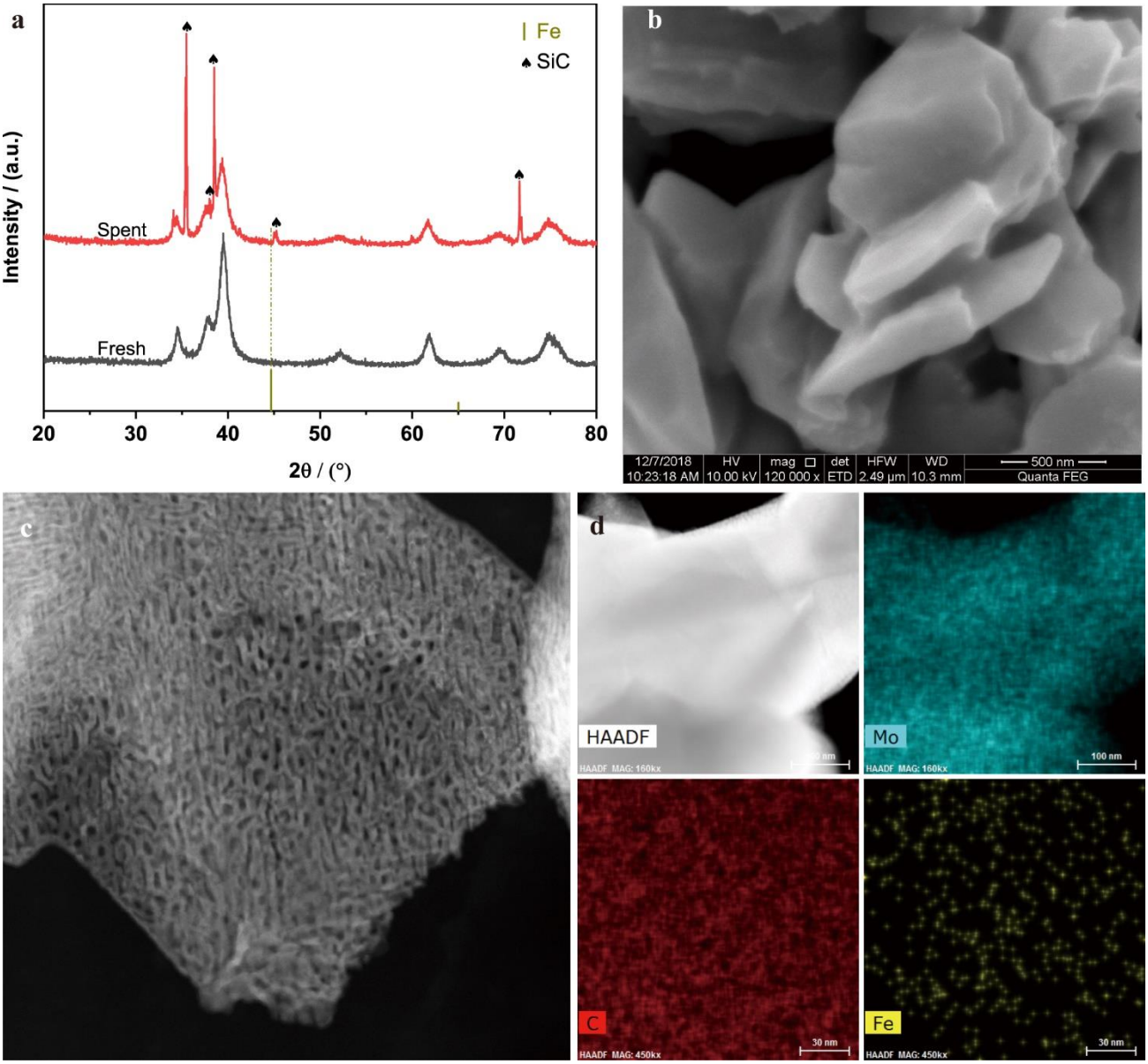

Figure S5. (a) XRD patterns of catalyst (1.5Fe-Mo_2C-600) before and after the reaction, (b) SEM image of spent catalyst (1.5Fe-Mo_2C-550), (c) STEM-HAADF image of spent catalyst (1.5Fe-Mo_2C-550), and (d) STEM image and corresponding STEM-EDX element mapping image of spent catalyst (1.5Fe-Mo_2C-550).

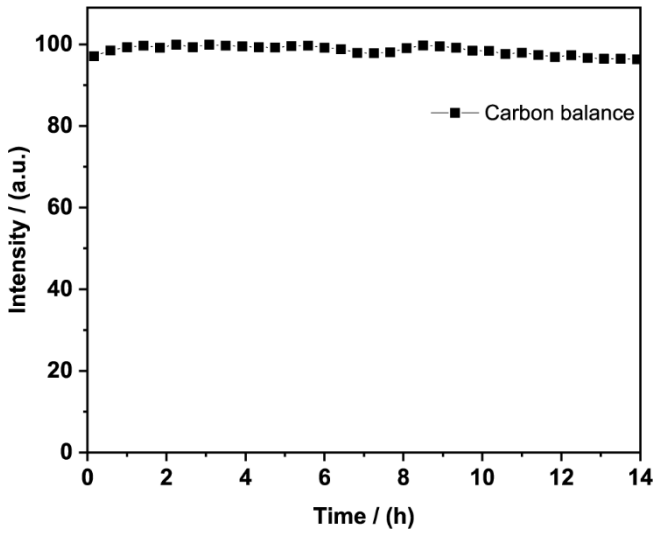

Figure S6. Carbon balance curve of during toluene hydrogenation using 1.5Fe-Mo_2C-550 as catalyst. (3.0 MPa of total pressure, 100 °C as reaction temperature, 0.15 h^{-1} as WHSV, employing newly synthesized Fe-doped molybdenum carbide catalysts).

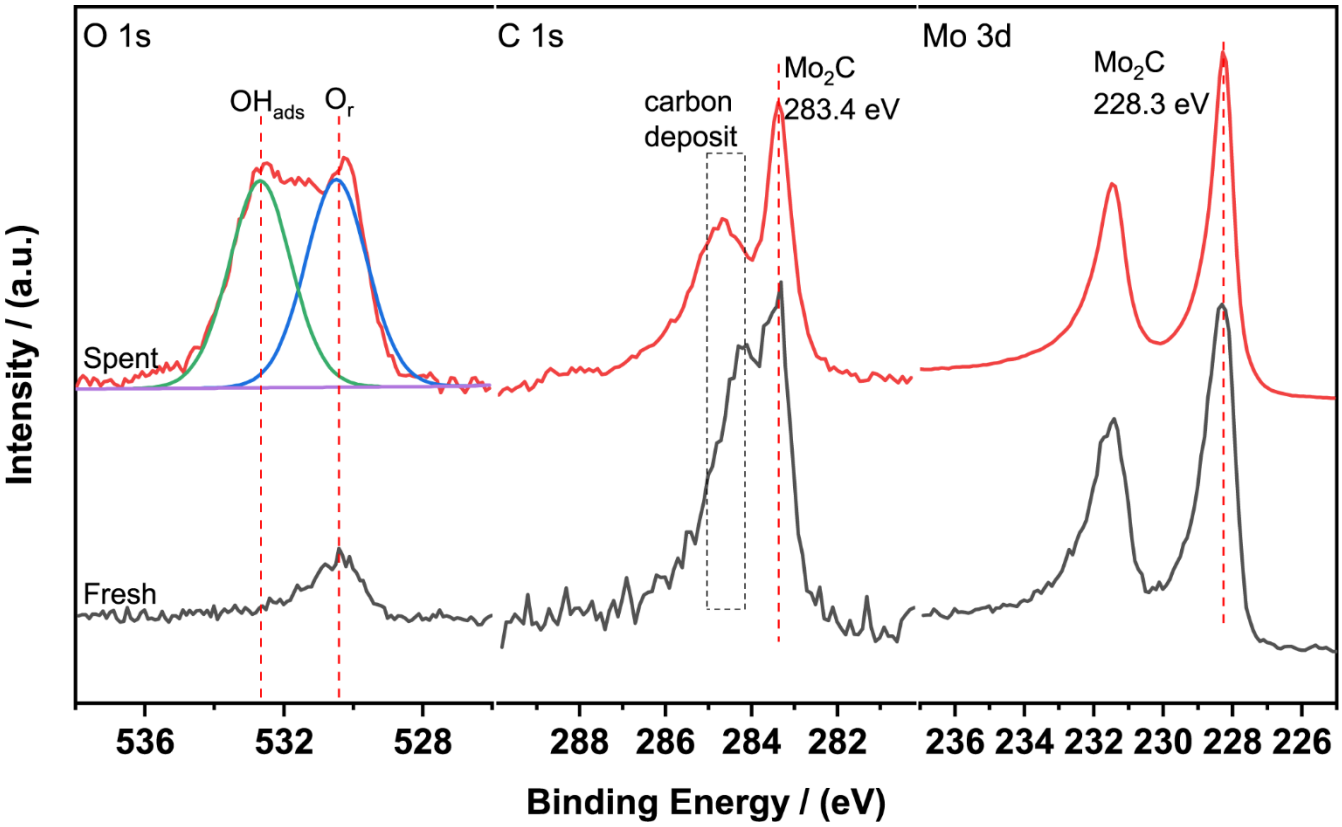

Figure S7. A control experiment using catalyst of 1.5Fe-Mo2C-550 for examining if surface of molybdenum carbide should be oxidized during transferring. The 1.5Fe-MoO_3 precursor was carburized in a fixed bed, which is identical one to the equipment used in toluene hydrogenation, at an atmosphere of 20% CH_4/H_2. After carburization, the reactor was sealed under pure N_2 atmosphere and consecutively transferred to glove box. The catalyst was pressed to a slice of 6 mm diameter in the glove box, and then the as-prepared sample was transferred to another glove box connected with XPS equipment load section using a sealed container avoiding the oxidation of catalyst by air. After that, the sample was loaded, vacuumed to UHV and transferred to analytic room for quasi in-situ XPS characterization.