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Gasification of metal-containing coals and carbons *via* their reaction with carbon dioxide

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Table S1 Properties of the activated coal CKT-6A used in the catalytic reactions.

Fraction/mm	*d* (bulk)/g cm^{-3}	Water capacity/ cm^3 g^{-1}	Specific surface area/m^2 g^{-1}(BET)	Pore volume/ cm^3 g^{-1}
0.2–0.45	0.42	0.66	1269	0.66

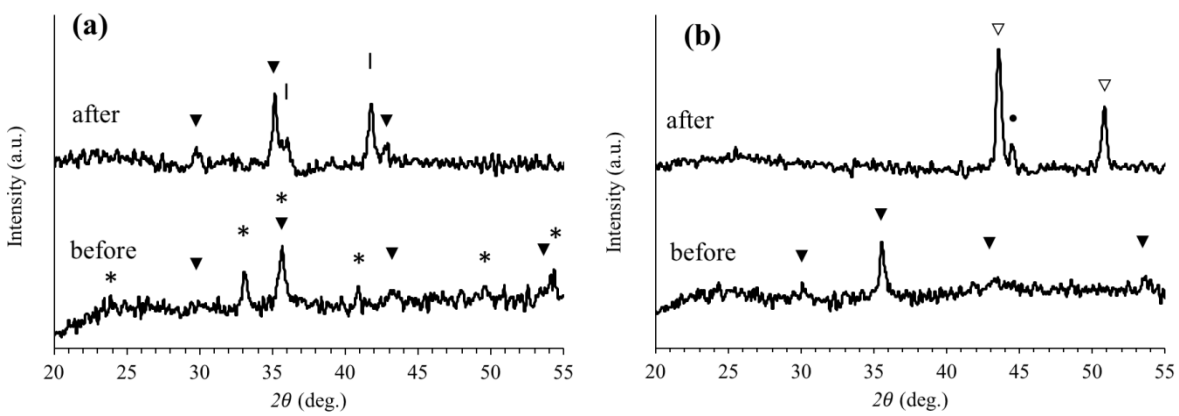

Figure S1 XRD patterns of (*a*) Fe/C(T) and (*b*) Fe/C(MW) samples before and after the catalytic reaction. The reflections of crystallographic planes for the specific iron compounds are indicated by the following symbols: * – Fe_2O_3; ▼ – Fe_3O_4; | – FeO; ▽ – Fe_3C; ● – Fe^0.

The initial Fe/C(T) sample contains a mixture of iron oxides [Figure S1(*a*)]. The predominant Fe_2O_3 phase demonstrates the peaks at 24.15 °, 33.16 °, 35.63 °, 40.86 °, 49.47 °, and 54.08 ° corresponding to the (012), (104), (110), (113), (024), and (116) crystallographic planes, respectively (JCPDS card No. 86-0550). The reflections at 30.08 °, 35.43 °, 43.05 °, and 53.41 ° are related to the (220), (311), (400), and (422) planes of magnetite, Fe_3O_4 (JCPDS card No. 82-1533). The initial Fe/C(MW) sample [Figure S1 (*a*)] contained only the Fe_3O_4 phase unlike the Fe/C(T) sample.

The average crystallite size (D_p) of oxide phases was calculated by the Debye-Scherrer equation:

$$D_p = 0.94\lambda/\beta\cos\theta,$$

where λ is the wavelength of CuKα irradiation, 1.54060 Å; β is the full width at the half maximum (FWHM) of the most intense reflection at 35.4° corresponding to the (311) plane of Fe_3O_4; and θ is the angle of diffraction. The average crystallite sizes are 7–8 nm and 10–12 nm for the initial Fe/C(T) and Fe/C(MW) samples, respectively.

The reduction of initial oxide phases occurs during the high-temperature catalytic reaction (see Figure S1). Carbon monoxide generated during this reaction acts as a reducing agent. The mixture of initial iron oxides (Fe_3O_4 and Fe_2O_3) transforms into Fe_3O_4 and FeO phases [see Figure S1(*a*)]. FeO (wüstite) manifests peaks at 35.77 ° and 41.54 ° corresponding to the (111) and (200) crystallographic planes, respectively (JCPDS card No. 79-1973). The XRD data [see Figure S1(*b*)]confirms that the Fe/C(MW) sample is subjected to stronger reduction during the catalytic process into Fe^0 with the reflection at 44.6 º (JCPDS card No. 06-0696) and forms the carbide phase (reflections at 43.60 º and 55.88 º), which is in agreement with the JCPDS card No. 85-0871.