

Electronic Supplementary Information (ESI)

Selective synthesis of α -Fe₂O₃ thin films and effect of the deposition temperature and lattice oxygen on the catalytic combustion of propene

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Table ESI 1 Experimental conditions for the preparation of α -Fe₂O₃

Precursor	Fe(acac) ₃
Solvent	Tetrahydrofuran
Concentration of precursor	5 mM
Frequency	4 Hz
Opening time	2 ms
Evaporation temperature	220 °C
Transportation temperature	220 °C
Substrate temperature	350 °C; 400 °C and 450 °C
Deposition pressure (mbar)	25
N ₂ (SLM)	0.16
O ₂ (SLM)	1.0
Substrates	Silicon, planar and mesh of stainless steel

Table ESI 2 Overview of the catalytic performance of the as-prepared α -Fe₂O₃ and some catalysts in the literature

Material	Weight (mg)	Gas composition	WHSV ^a (ml g ⁻¹ h ⁻¹)	T ₁₀ ^b (°C)	T ₅₀ ^b (°C)	T ₉₀ ^b (°C)	Ref.
α -Fe ₂ O ₃ 350 °C	20	1% C ₃ H ₆ /10% O ₂ in Ar	45000	260	313	350	This work
α -Fe ₂ O ₃ 400 °C				295	355	400	
α -Fe ₂ O ₃ 450 °C				302	380	435	
Co ₃ O ₄	12	1% C ₃ H ₆ /10% O ₂ in Ar	75000	306	347	396	[1]
Co ₃ O ₄	41.5	2% C ₃ H ₆ / 20%O ₂ in Ar	73000	293	327	356	[2]
Co ₃ O ₄	12	2% C ₃ H ₆ / 20%O ₂ in Ar	75000	325	354	385	[3]
Co _{2.66} Mn _{0.34} O ₄	12	2% C ₃ H ₆ / 20%O ₂ in Ar	75000	277	321	356	[3]
Cu _{0.72} Co _{2.28} O ₄	40	13% C ₃ H ₆ / 52%O ₂ in N ₂	15000	230	275	>400	[4]
Au/Al ₂ O ₃	200	1.5% C ₃ H ₆ / 4% O ₂ in He	22500	288	349	410	[5]
Au/Al ₂ O ₃	200	1% C ₃ H ₆ / 9% O ₂ in He	219512	-	365	-	[6]
Au/BaO/Al ₂ O ₃	200	1% C ₃ H ₆ / 9% O ₂ in He	250000	-	290	-	[6]
Au/Rb ₂ O/Al ₂ O ₃	200	1% C ₃ H ₆ / 9% O ₂ in He	257143	-	307	-	[6]
Au/Li ₂ O/Al ₂ O ₃	200	1% C ₃ H ₆ / 9% O ₂ in He	225000	-	327	-	[6]
Au/MgO/Al ₂ O ₃	200	1% C ₃ H ₆ / 9% O ₂ in He	214286	-	359	-	[6]
Ag/Al ₂ O ₃	50	3% C ₃ H ₆ / 10% O ₂ in N ₂	12000	-	-	420	[7]
La _{1.7} Sr _{0.3} CuO ₄ S _{0.2}	200	0.1% C ₃ H ₆ / 5% O ₂ in N ₂	30000	368	419	500	[8]
Non-coated mesh	-	1% C ₃ H ₆ /10% O ₂ in Ar	-	381	550	680	This work

Note: ^a WHSV is weight hourly space velocity; ^b T₁₀, T₅₀ and T₉₀ refer to the temperatures at which 10%, 50% and 90% propene is converted, respectively.

The table ESI 2 presents an overview of the catalytic performance of the as-prepared α -Fe₂O₃ and selected catalysts in the literature. Special attention is devoted to the comparison of the catalytic performance with noble metals and transition metals oxides. As crucial factors, the weights of the catalyst and the WHSV have been taken in account. Even though the experimental conditions are somewhat different, it can be seen from the table that both groups give similar results with the respect to the oxidation of propene. As pointed out in our recent work, Co₃O₄ and Co-based mixed oxide are very active. Up to now, only few studies involved iron oxide, especially hematite, for propene conversion. As mentioned in the introduction, iron compounds are abundantly available

and have attractive consideration attention because of their properties such as high thermodynamic stability and low cost; also, they are environmentally friendly. Therefore, α -Fe₂O₃ presents significant advantages over others transition metal oxides. In summary, as demonstrated here, hematite investigated in the present study can be successfully synthesized and is very active for VOCs conversion.

Carbon species analysis

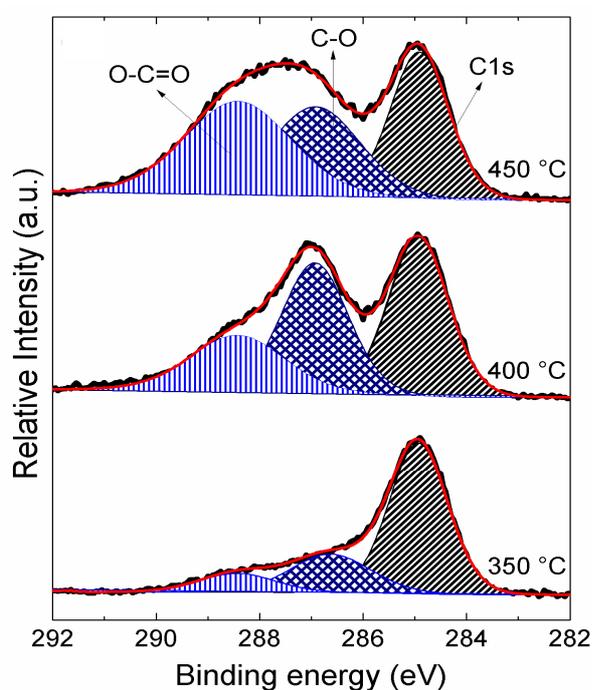


Fig. ESI 1 XPS spectra of C1s core shell present on α -Fe₂O₃. Thin and thick lines are fitted and experimental results, respectively.

Figure ESI 1 shows the C1s signal, in which three observed peaks are resolved into three components corresponding to adventitious carbon, C–O, and O–C=O moieties, respectively. The observed peaks confirmed the presence of a large amount amount of carbonaceous species at the surface of the as-prepared α -Fe₂O₃, which are in excellent agreement with results of the oxygen signals.

Comparison of XPS results of hematite samples before and after the catalytic test

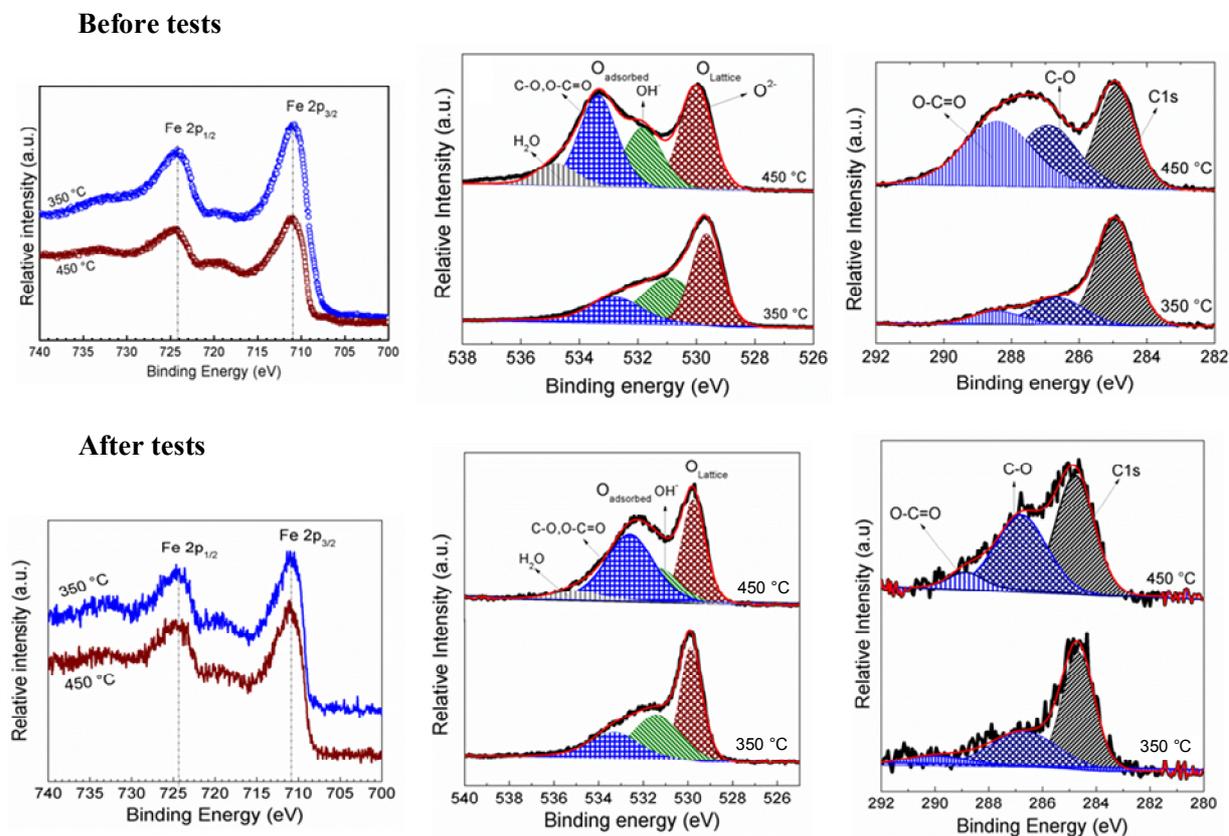


Fig. ESI 3 XPS spectra of hematite prepared at 350 °C and 450 °C before and after the catalytic tests. The high noise in the “after tests” measurements was due to a substantially lower X-ray source intensity.

As can be seen from Figs. ESI 2 and 3, the film morphology and surface composition remain quite similar for the samples before and after the catalytic test. Together with the reproducibility results in Fig. 8b, it can be predicted that the catalytic properties are not largely affected, which is also supported by the present morphology and composition results.

Brief description of the PSE-CVD reactor

The growth of $\alpha\text{-Fe}_2\text{O}_3$ thin films was performed in a cold-wall stagnation point-flow CVD reactor, which is associated with a homemade PSE unit for the control delivery of liquid precursor feedstock. The reactor consists of three detachable parts: the evaporation zone (part I), carrier and transport gas zone (Part II) located above the cold-wall CVD chamber in which a flat heater (part III) is placed over the ceramic blocks. All parts were heated separately, and their temperatures were controlled by a temperature control unit (HT-60, Horst).

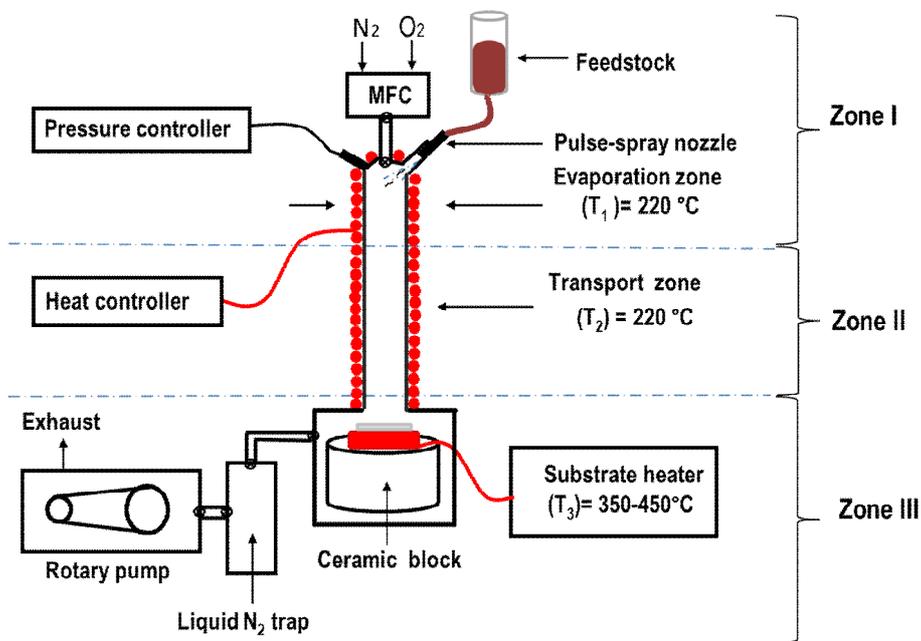


Fig. ESI 4 PSE-CVD reactor used for the synthesis of hematite.

Flow reactor use for the catalytic test

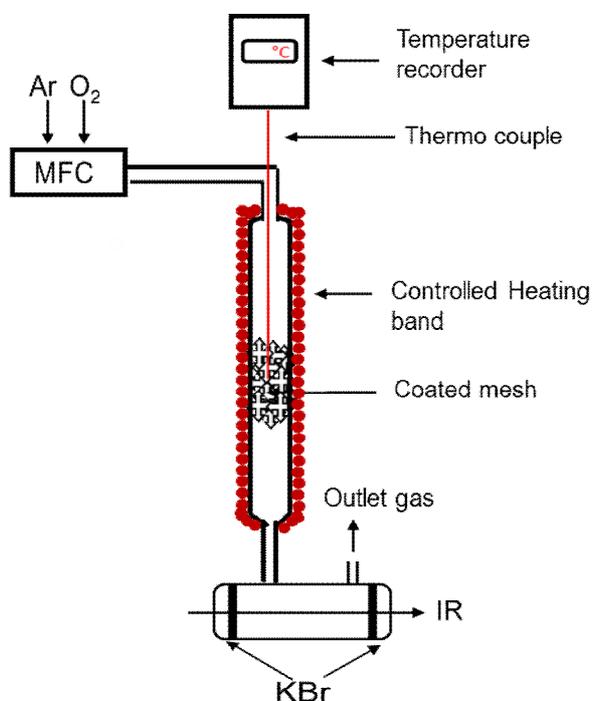


Fig. ESI 5 Schematic representation of the flow-reactor used for catalytic test.

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