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负载型Rh基催化剂上的CO加氢制乙醇反应：载体效应

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CO Hydrogenation to Ethanol over Supported Rh-Based Catalyst: Effect of the Support

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Table S1 Performance of CO hydrogenation over various catalysts [a].

Catalyst	X_{CO}[b]/%	Selectivity (%)			Alcohol distribution (*w*, %)				
		ROH [c]	CH_n [d]	CO_2	MeOH	EtOH	PrOH	BuOH	C_{5+} OH
$RhFe/CeO_2$	5.1	25.6	71.3	3.1	60.2	30.1	7.8	1.5	0.4
$RhFe/ZrO_2$	7.2	27.8	70.7	1.6	52.5	39.4	6.5	1.3	0.3
$RhFe/TiO_2$	18.2	33.2	62.4	4.4	15.6	74.7	4.3	5.2	0.2
Fe/TiO2	1.4	–	> 99.9	–	–	–	–	–	–

[a] Reaction conditions: $H_2/CO = 2$, 250 ºC, 2 MPa, 40 mL·min^{-1}, TOS = 48 h.

Table S2 ICP-OES and XPS results, surface species content for different catalysts.

Catalyst	Loading (*w*, %)		Surface atomic percentage [a]		Surface species content [b] (*w*, %)	
	Rh	Fe	Rh^0	Rh^+	Rh^0	Rh^+
$RhFe/CeO_2$	2.0	3.9	307.1(77.9%)	308.8(22.1%)	0.31	0.09
$RhFe/ZrO_2$	2.3	3.9	307.2(66.0%)	308.9(34.0%)	0.37	0.19
$RhFe/TiO_2$	2.1	4.2	307.1(52.4%)	308.9(47.6%)	0.54	0.49

[a] Estimated by XPS spectrum fitting result of Rh 3*d* in different catalyst. [b] Estimated by actual loading, metal dispersion and the percentage of Rh^0 and Rh^+.

Table S3 Surface atomic ratio estimated by XPS for different catalysts.

Catalyst	Ratio
	$O_{II}/(O_I + O_{II} + O_{III})$
$RhFe/CeO_2$	0.21
$RhFe/ZrO_2$	0.22
$RhFe/TiO_2$	0.40

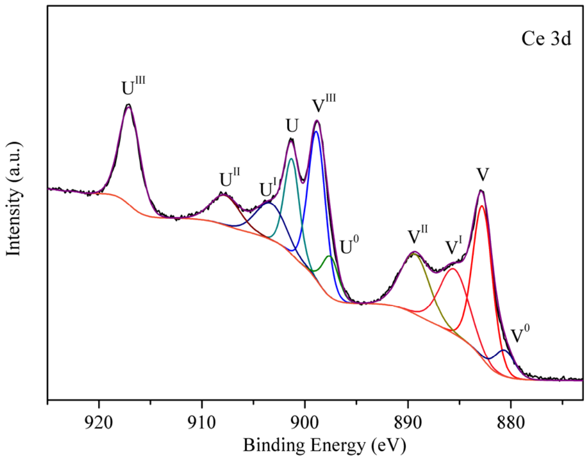

Fig. S1 Ce 3*d* region of $RhFe/CeO_2$.

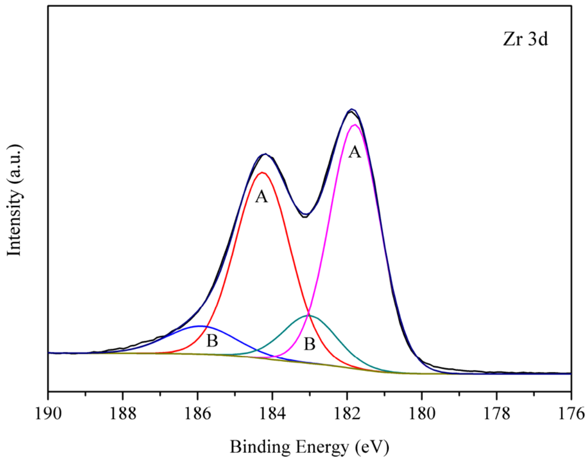

Fig. S2 Zr 3*d* region of $RhFe/ZrO_2$.

The peaks of Ce 3$d_{5/2}$ and Ce 3$d_{3/2}$ in Fig. S1 labeled as V, V^{II}, V^{III} and U, U^{II}, U^{III} corresponded to unreduced Ce^{4+}, V^0, V^I, U^0 and U^I were features of Ce^{3+} [1]. Partial reduction of Ce^{4+} and formation of oxygen vacancies on RhFe/CeO_2 could be achieved during XPS pretreatment in a vacuum, in accordance with the viewpoint of Fierro *et al.* [2]. On Fig. S2, the spectrum of Zr 3d was deconvolved into two parts (A and B), which were characteristic for unreduced Zr^{4+} [3]. Thus, it was inferred that a little bit of O_{II} in RhFe/ZrO_2 should be due to the interaction between metal and support.

References

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