ESI for

Direct dehydrogenation of isobutane to isobutene over Zn-doped ZrO_2 metal oxide heterogeneous catalysts

Yang Liu, Chengjie Xia, Qi Wang, Lei Zhang, Ao Huang, Ming Ke* and Zhaozheng Song

State Key Laboratory of Heavy Oil Processing, China University of Petroleum (Beijing), Beijing 102249, PR China.

Corresponding Author:

keming@cup.edu.cn or keming_cup@126.com (M. Ke)

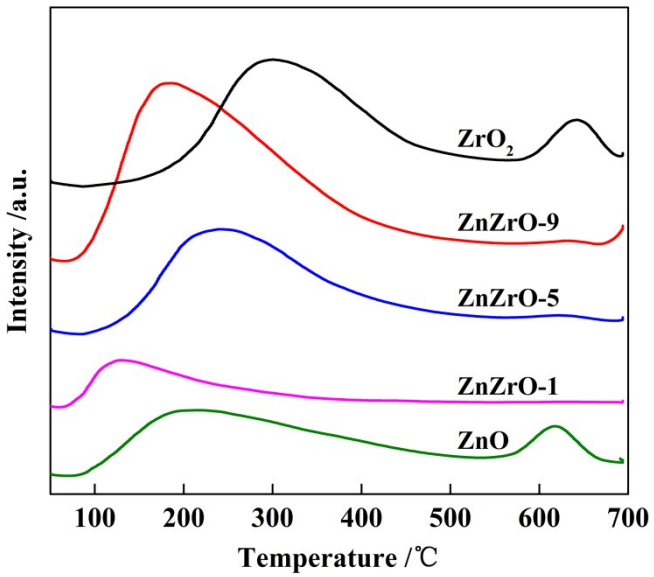


Fig. S1 CO_2-TPD curves of ZnO, ZnZrO-*x*, and ZrO_2.

Table S1 Surface basicity of investigated catalysts.

Catalyst	Temperature of maximum /°C	Quantity of basic sites /mmol g^{-1}	Total basic sites /mmol g^{-1}
ZrO_2	298	0.1873	0.2070
	642	0.0184	
ZnZrO-9	183	0.2763	0.2788
	634	0.0008	
ZnZrO-5	239	0.1615	0.1648
	631	0.0023	
ZnZrO-1	128	0.0715	0.0721
	624	0.0002	
ZnO	200	0.1139	0.1287
	619	0.0142	

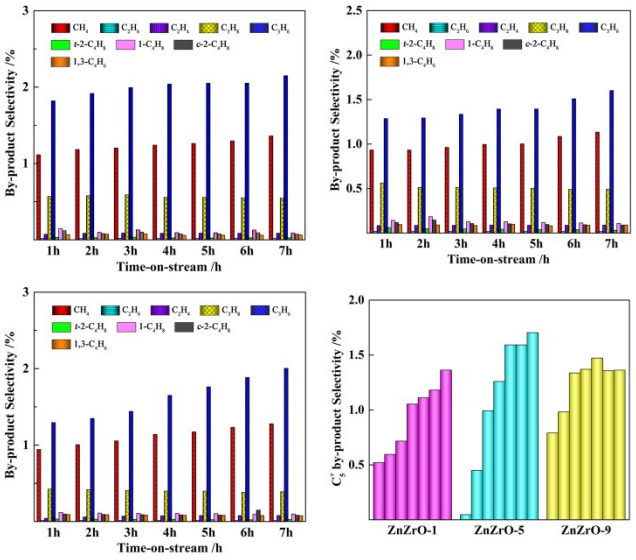


Fig. S2 By-product selectivity of (a) ZnZrO-1, (b) ZnZrO-5, and (c) ZnZrO-9, (d) C_5^+ by-products selectivity of three ZnZrO-*x* mixed oxides.

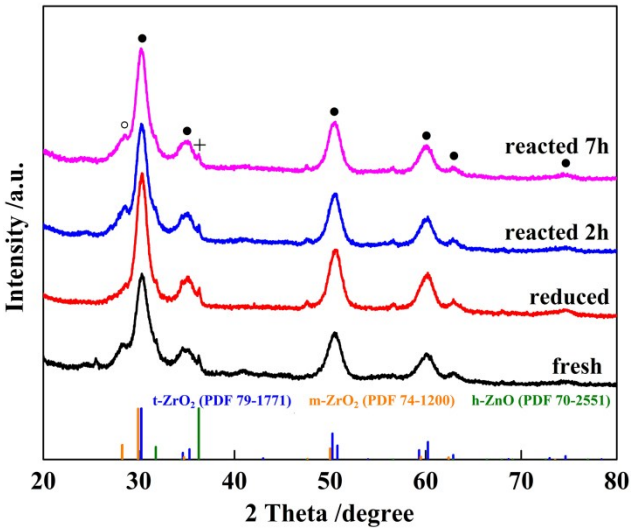
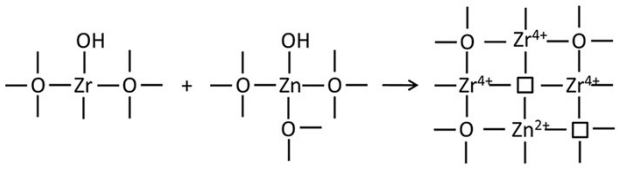


Fig. S3 XRD patterns of (a) ZnO, (b) ZnZrO-1, (c) ZnZrO-5, (d) ZnZrO-9 and (e) ZrO_2. (+: *h*-ZnO, •: *t*-ZrO_2, o: *m*-ZrO_2).



Scheme S1 The formation of Zr^{4+}_{cus} sites and oxygen vacancies.

Table S2 Surface and bulk Zr/Zn atom ratio of ZnZrO-5 from XPS and EDX.

Sample	Scan spot	Atomic /%			Zr/Zn mole ratio
		Zr	Zn	O	
XPS	1	8.14	18.55	73.31	2.28
	2	8.01	20.42	71.56	2.54
EDX	1	4.39	22.13	73.48	5.04
	2	5.41	26.46	68.14	4.90