## **Supporting Information**

## Structure-Activity-Selectivity Relationships in Propane Dehydrogenation over Rh/ZrO<sub>2</sub> Catalysts

Yaoyuan Zhang<sup>1,2†</sup>, Yun Zhao<sup>1†</sup>, Tatiana Otroshchenko<sup>1</sup>, Anna Perechodjuk<sup>1</sup>, Vita A.

Kondratenko<sup>1</sup>, Stephan Bartling<sup>1</sup>, Uwe Rodemerck<sup>1</sup>, David Linke<sup>1</sup>, Haijun Jiao<sup>1,\*</sup>, Guiyuan

Jiang<sup>2,\*</sup>, Evgenii V. Kondratenko<sup>1,\*</sup>

<sup>1</sup>Leibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Straße 29a,

Rostock, 18059, Germany

<sup>2</sup>State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing, Beijing,

102249, China

\*Correspondence to: evgenii.kondratenko@catalysis.de (E.V.K.); jianggy@cup.edu.cn (G.J.); hajiun.jiao@catalysis.de (H.J.)

*†*These authors contributed equally to this work.

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Catalysts	Zr / at.%	O / at.%	C / at.%	F / at.%
ZrO <sub>2</sub>	31.6	56.6	8.5	3.3
$0.01 Rh/ZrO_2$	31.9	61.3	6.8	-
$0.05 Rh/ZrO_2$	32.0	56.5	7.6	3.9
0.2Rh/ZrO <sub>2</sub>	30.0	57.5	10.3	2.2

**Table S1.** Surface element composition for differently loaded Rh/ZrO<sub>2</sub> catalysts calculated from survey scan XP spectra.

x	$E_{\rm coh}/{\rm eV}$	Rh <sub>x</sub> Sites	
1	-3.17	Figure S6(a)	
4	-3.83	Figure S6(b)	
	-3.92	Figure S6(c)	
	-3.67	Figure S6(d)	
10	-4.40	Figure S6(e)	
	-4.37	Figure S6(f)	

**Table S2.** The cohesive energy per Rh atom of the  $Rh_x/ZrO_2(-111)$  (*x*=1, 4 and 10).

x	N of O <sub>v</sub>	$E_{\rm r}/{\rm eV}$
0	$1O_v$	3.17
	$1O_{\rm v}$	0.85
1	$2O_{\rm v}$	1.45
	30 <sub>v</sub>	3.14
	$1O_v$	-0.16
4	$2O_{\rm v}$	0.90
	30 <sub>v</sub>	1.33
	$1O_{\rm v}$	0.43
	$2O_{\rm v}$	1.07
10	$3O_{\rm v}$	1.21
10	$4O_{\rm v}$	1.38
	$5O_{\rm v}$	2.00
	6O <sub>v</sub>	2.04

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