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Electronic Supplementary Information

A size-selective method for increasing the performance of Pt supported on tungstated zirconia catalysts for alkanes isomerization: a combined experimental and theoretical DFT study

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Table S1. Results of Rietveld analysis using Jade 2020.

Sample	Phases	Cell parameters (A)			Cell volume ($Å^3$)	Phase concentration wt. %	Crystall size (nm)
		a_0	b_0	c_0			
WZ15-7	T-ZrO_2	3.5980	3.5980	5.3672	69.5	87.2	11.7
	M-ZrO_2	5.1505	5.2116	5.3173	142.7	7.3	
	M-WO_3	7.3090	7.5220	7.6780	422.1	5.4	
WZ15-H7	T-ZrO_2	3.5985	3.5985	5.1873	67.2	81.4	10.8
	M-ZrO_2	5.1525	5.2074	5.3277	142.9	10.8	
	M-WO_3	7.3090	7.5220	7.6780	422.1	7.8	
WZ20-7	T-ZrO_2	3.5960	3.5960	5.1952	67.2	83.8	11.2
	M-ZrO_2	5.1505	5.2116	5.3173	142.7	7.7	
	M-WO_3	7.3090	7.5220	7.6780	422.1	8.5	
WZ20-7H	T-ZrO_2	3.5983	3.5983	5.1940	67.3	81.2	11.4
	M-ZrO_2	5.1505	5.2116	5.3173	142.7	14	
	M-WO_3	7.3090	7.5220	7.6780	422.1	4.8	
WZ15-8	T-ZrO_2	3.5964	3.5964	5.1968	67.2	81.6	14.5
	M-ZrO_2	5.1505	5.2116	5.3173	142.7	12.3	
	M-WO_3	7.3090	7.5220	7.6780	422.1	6.1	
WZ15-H8	T-ZrO_2	3.5964	3.5964	5.1968	67.2	81.6	16
	M-ZrO_2	5.1505	5.2116	5.3173	142.7	12.3	
	M-WO_3	7.3090	7.5220	7.6780	422.1	6.1	
WZ20-8	T-ZrO_2	3.5965	3.5965	5.1988	67.2	72.2	15.3
	M-ZrO_2	5.1505	5.2116	5.3173	142.7	14.7	
	M-WO_3	7.3090	7.5220	7.6780	422.1	13.1	
WZ20-H8	T-ZrO_2	3.5915	3.5915	5.1905	67.0	76	14.9
	M-ZrO_2	5.1505	5.2116	5.3173	142.7	17.9	
	M-WO_3	7.3090	7.5220	7.6780	422.1	6.1	

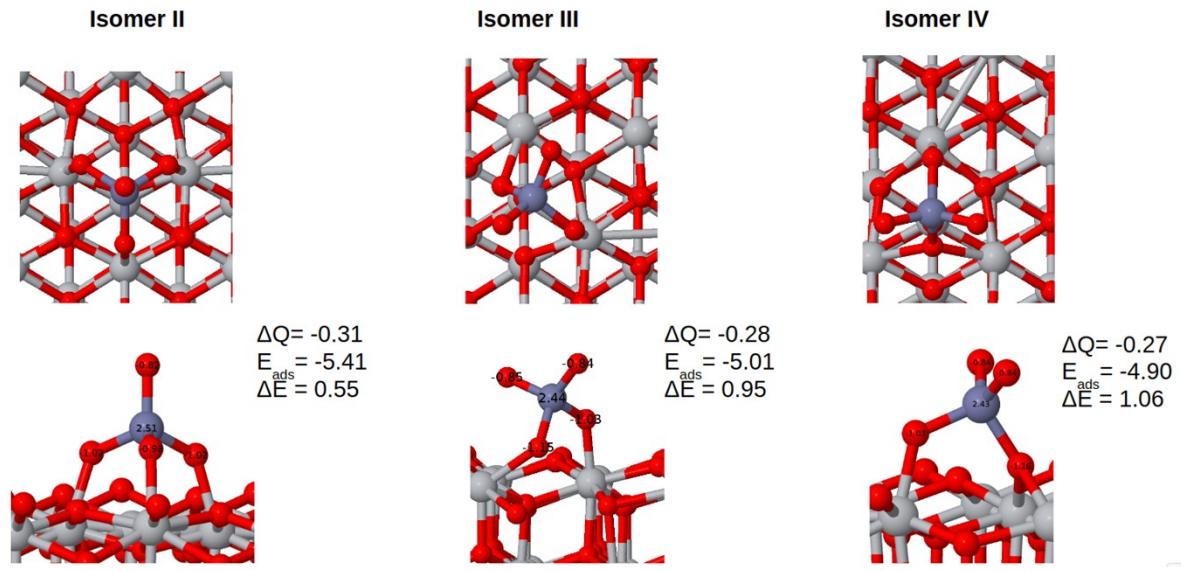

Figure S1. Top and side view of the local minima found for the WO_3/ZrO_2 system, along with the total Bader charge on the $(WO_3)_x$ (ΔQ), adsorption energies to the support (E_{ads}), and energy difference of each isomer with respect to the putative global minima (ΔE), in eV. Bader charges are depicted on the atoms. W, O, and Zr atoms are shown in purple, red, and grey, respectively.

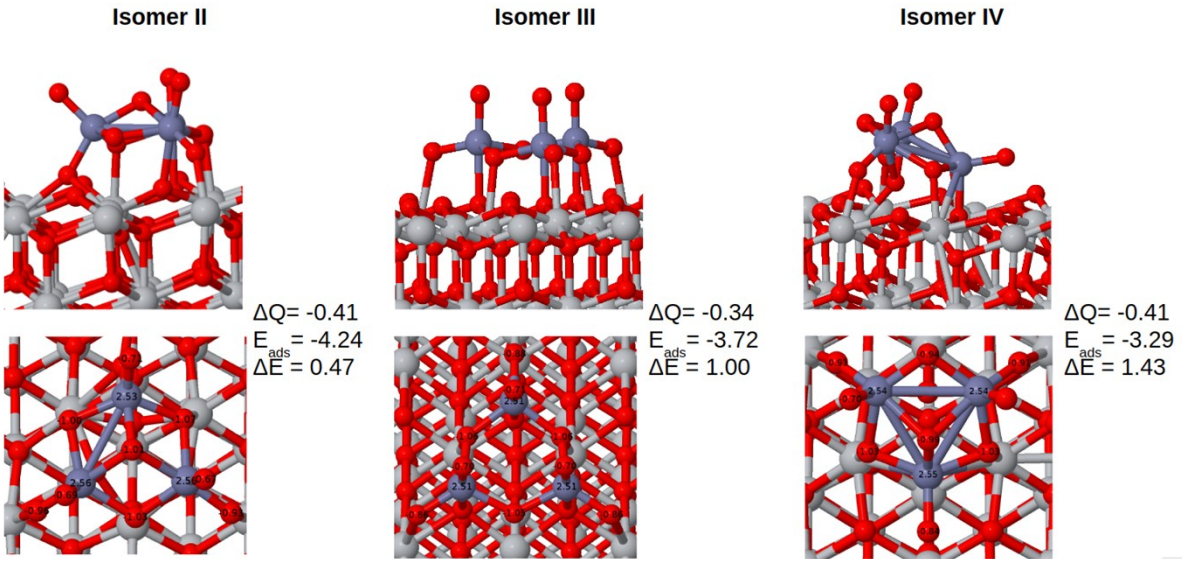

Figure S2. Side and top view of the local minima found for the $(WO_3)_3/ZrO_2$ system, along with the total Bader charge on the $(WO_3)_x$ (ΔQ), adsorption energies to the support (E_{ads}), and energy difference of each isomer with respect to the putative global minima (ΔE), in eV. Bader charges are depicted on the atoms. W, O, and Zr atoms are shown in purple, red, and grey, respectively.

The surface tungsten density is a common synthesis parameter reported for tungstated zirconia catalysts, assuming all tungsten is on the surface. In this work it was calculated following the formula reported for Naito et al. [1], as follows:

Surface tungsten density (W atom/nm^2) = [WO_3 loading (wt.%)/100]/231.8 (formula weight of WO_3) · 6.023 x 10^{23} / [BET surface area (m^2 g^{-1}) x 10^{18}].

[1] "Tungsten oxide monolayer loaded on zirconia: determination of acidity generated on the monolayer", N. Naito, N. Katada and M. Niwa*, J. Phys. Chem*, 1999, **103**, 7206.