SUPPORTING INFORMATION

An in-depth simulation analysis of the reaction mechanism of ethanol dehydration to ethylene and carbon deposition on the γ-Al_2O_3(100) surface

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Table S1. Changes in structural parameters of ethanol on the γ-Al_2O_3(100) surface

Structural parameters	Ethanol	
	Before adsorption	After adsorption
d(C1-C2)/Å	1.51	1.50
d(C1-H2)/Å	1.08	1.07
d(C1-H3)/Å	1.08	1.07
d(C2-H4)/Å	1.10	1.08
d(C2-H5)/Å	1.08	1.08
d(C2-H6)/Å	1.08	1.07
d(C1-O)/Å	1.45	1.48
d(O-H1)/Å	0.97	0.98
∠(H1-O-C1)/°	109.26	110.57
∠(H2-C1-C2)/°	109.85	111.07
∠(C2-C1-O)/°	109.10	111.05
∠(H4-C2-C1)/°	111.04	111.68
∠(H5-C2-C1)/°	110.64	111.13
∠(H6-C2-C1)/°	110.45	109.43
∠(O-C1-C2)/°	112.66	111.05
∠(H2-C2-H3)/°	107.28	108.99
∠(H3-C1-C2)/°	109.77	110.94
∠(H4-C2-H5)/°	108.24	108.24
∠(H4-C2-H6)/°	108.22	108.24
∠(H5-C2-H6)/°	108.16	108.01

Table S2. Changes in structural parameters of water on the γ-Al_2O_3(100) surface

Structural parameters	Water	
	Before adsorption	After adsorption
d(H1-O)/Å	0.97	0.98
d(H2-O)/Å	0.97	0.97
∠(H1-O-H2)/°	106.03	106.36

Table S3. Changes in structural parameters of ether on the γ-Al_2O_3(100) surface

Structural parameters	Ether	
	Before adsorption	After adsorption
d(C1-C2)/Å	1.51	1.50
d(C3-C4)/Å	1.51	1.51
d(C2-O)/Å	1.44	1.47
d(C3-O)/Å	1.44	1.47
d(C1-H1)/Å	1.08	1.07
d(C1-H2)/Å	1.08	1.07
d(C1-H3)/Å	1.10	1.08
d(C2-H4)/Å	1.08	1.07
d(C3-H6)/Å	1.08	1.07
∠(H1-C1-H2)/°	108.13	108.56
∠(H1-C1-H3)/°	108.30	108.50
∠(H2-C1-H3)/°	108.16	107.51
∠(H1-C1-C2)/°	110.94	111.24
∠(H2-C1-C2)/°	110.52	109.54
∠(H3-C1-C2)/°	110.70	111.38
∠(H4-C2-C1)/°	110.12	111.68
∠(H5-C2-C1)/°	110.21	111.13
∠(O-C2-C1)/°	109.42	112.90
∠(C2-O-C3)/°	112.34	114.65
∠(O-C3-C4)/°	109.39	112.01
∠(H4-C2-O)/°	110.04	107.95
∠(H5-C2-O)/°	110.06	107.41
∠(H4-C2-H5)/°	106.97	107.77
∠(H8-C4-H9)/°	108.06	108.25
∠(H8-C4-H10)/°	108.19	107.82

Table S4. Changes in structural parameters of ethane on the γ-Al_2O_3(100) surface

Structural parameters	Ethane	
	Before adsorption	After adsorption
d(C1-C2)/Å	1.52	1.52
d(C1-H1)/Å	1.08	1.08
d(C1-H2)/Å	1.08	1.08
d(C1-H3)/Å	1.08	1.08
d(C2-H3)/Å	1.08	1.08
d(C2-H4)/Å	1.08	1.08
d(C2-H5)/Å	1.08	1.08
d(C2-H6)/Å	1.08	1.08
∠(H1-C1-C2)/°	111.50	111.29
∠(H2-C1-C2)/°	111.52	111.67
∠(H3-C1-C2)/°	111.51	111.24
∠(H1-C1-H2)/°	107.32	107.60
∠(H1-C1-H2)/°	107.44	107.42
∠(H1-C1-H3)/°	107.32	107.40

Table S5. Changes in structural parameters of ethylene on the γ-Al_2O_3(100) surface

Structural parameters	Ethylene	
	Before adsorption	After adsorption
d(C1-C2)/Å	1.32	1.32
d(C1-H1)/Å	1.07	1.07
d(C1-H2)/Å	1.07	1.07
d(C2-H3)/Å	1.07	1.07
d(C2-H4)/Å	1.07	1.07
∠(H1-C1-C2)/°	121.25	120.79
∠(H2-C1-C2)/°	121.25	121.08
∠(H3-C2-C1)/°	121.25	121.23
∠(H4-C2-C1)/°	121.25	120.81
∠(H1-C1-H2)/°	117.50	118.09
∠(H3-C2-H4)/°	117.50	117.96

Table S6. Changes in structural parameters of butene on the γ-Al_2O_3(100) surface

Structural parameters	Butene	
	Before adsorption	After adsorption
d(C1-C2)/Å	1.32	1.32
d(C1-H1)/Å	1.07	1.07
d(C1-H2)/Å	1.07	1.07
d(C2-H3)/Å	1.07	1.07
d(C2-C3)/Å	1.49	1.07
d(C3-H4)/Å	1.08	1.08
d(C3-H5)/Å	1.08	1.08
d(C4-H6)/Å	1.08	1.08
d(C4-H7)/Å	1.08	1.08
d(C4-H8)/Å	1.08	1.08
d(C3-C4)/Å	1.53	1.52
∠(H1-C1-H2)/°	118.17	118.82
∠(H1-C1-C2)/°	121.14	121.55
∠(H2-C1-C2)/°	120.69	119.31
∠(H3-C2-C1)/°	118.14	117.57
∠(C1-C2-C3)/°	125.34	125.34
∠(C2-C3-H4)/°	109.39	108.27
∠(H4-C3-H5)/°	106.41	105.30
∠(C3-C4-H6)/°	111.10	111.21
∠(C3-C4-H7)/°	111.25	111.21
∠(C3-C4-H8)/°	110.92	112.62
∠(H6-C4-H7)/°	107.66	106.42
∠(H6-C4-H8)/°	108.07	107.55
∠(H7-C4-H8)/°	107.67	107.56