Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information:

Insight into the mechanism of methanol assistance with syngas conversion over partially hydroxylated γ-Al_2O_3 (110D) surface in slurry bed

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Table S1 Structural parameters and adsorption energies of adsorbed H_2O in different configurations.

Configurations	E_{ads}/kJ mol^{-1}	Al–O_{water} bond/Å	$O_{surface}$–H bond/Å	O_{water}–H bond/Å
(110D)-1×1-H_2O (b)	196.3	1.73	1.00	0.97
(110D)-1×1-H_2O (b-1)	183.1	1.93	1.00	1.03
(110D)-1×1-H_2O (b-2)	182.6	1.73	1.01	0.97
(110D)-1×1-H_2O (b-3)	176.3	1.75	1.00	0.97
(110D)-1×1-H_2O (b-4)	164.1	1.74	0.99	0.97
(110D)-1×1-H_2O (b-5)	149.3	1.98	0.98	1.05
(110D)-1×1-2H_2O (c)	205.5	1.78	0.98	1.02

Figure S1 Top and side views of the optimized low-lying configurations of γ-Al_2O_3 (110D)-1×1surface with 1 H_2O adsorbed ($\theta_{OH}\approx$4.5 OH·nm^{-2}) in liquid paraffin, with their relative adsorption energies of H_2O in kJ·mol^{-1} indicated.

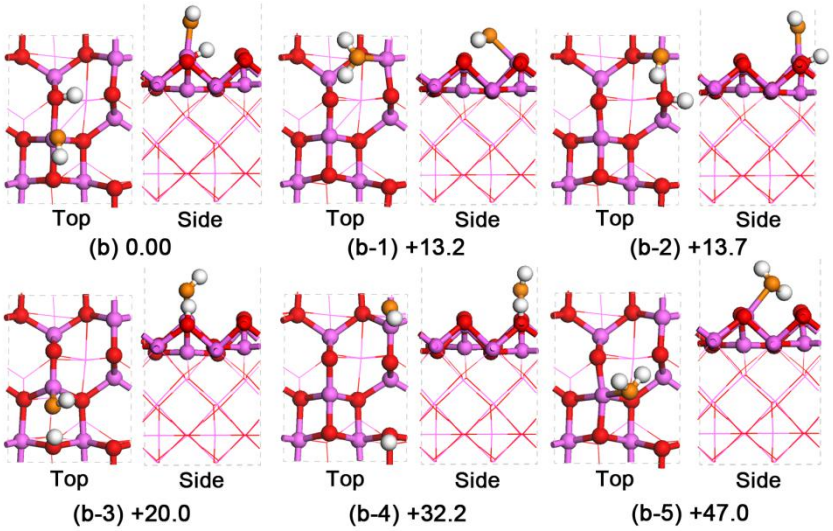

Figure S2 Potential energy diagram and the structures of initial states (IS), transition states (TS), and final states (FS) for (a) CH_4 and C_2H_6 formation and (b) CH_3OCH_3 formation and on the partially hydroxylated γ-Al_2O_3 (110D) surface in liquid paraffin. See Fig. 2 for color coding.