Revealing the synergetic effects between reactants in oxidative coupling of methane on stepped MgO(100) catalyst

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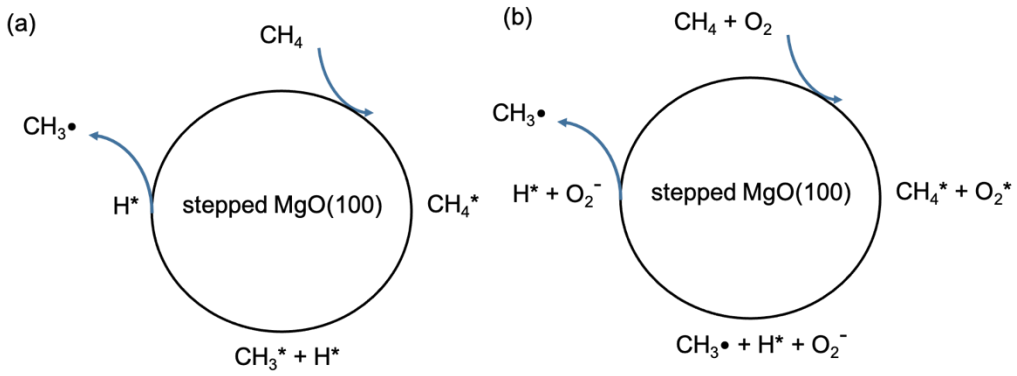
Table S1 The optimized bond distance and adsorption energies of CH_4 and O_2 molecular adsorbed on the Stepped MgO(100).

	O_2*	CH_4*	CH_4* + O_2*
E/eV	-0.25	-0.25	-0.38
R(C-H)/Å		1.10	1.10
R(O_s-H)/Å		2.50	2.30
R(C-Mg)/Å		2.86	
R(O-O)/Å	1.26	-	1.26
R(O-Mg)/Å	2.30 2.86	-	2.31 2.92
R(O_s-Mg)/Å	2.13 2.14	2.13 2.13	2.14 2.14

Table S2 The optimized bond distance and bader charge along the reaction pathway of the first C-H bond breaking on the Stepped MgO(100).

	Pathway I			Pathway II		
	CH_4*	TS	H* + CH_3*	CH_4* + O_2*	TS	O_2-* + H* + CH_3•
R(C-H)/Å	1.10	1.40		1.10	1.39	
R(O_s-H)/Å	2.50	1.28	0.99	2.30	1.21	0.98
R(C-Mg)/Å	2.86	2.26	2.18			
R(O-O)/Å	-	-	-	1.26	1.31	1.37
R(O-Mg)/Å	-	-	-	2.31 2.92	2.13 2.32	2.03 2.23
R(O_s-Mg)/Å	2.13 2.13	2.58 1.98	2.78 1.95	2.14 2.14	2.46 2.02	2.79 1.93
Q(Os)/*e*	-1.67	-1.65	-1.65	-1.56	-1.39	-1.63
Q(Mg)/*e*	1.63	1.63	1.64	1.64(-Os) 1.65 1.64	1.64(-Os) 1.66 1.64	1.65(-Os) 1.64 1.64
Q(O)/*e*				-0.16 -0.08	-0.28 -0.31	-0.48 -0.41
Q(H)/*e*	0.06	0.38	0.75	0.03	0.38	0.76
Q(CH_3)/*e*	-0.10	-0.55	-0.76	-0.05	-0.19	0.00



Scheme S1. The schematic illustration OCM reaction mechanism. (a) conventional MvK (b) proposed L-H.