Supporting Information

Mechanistic insights into the oxidative coupling of methane over Li/MgO catalyst: An experimental and microkinetic modeling study

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Table S1. The used photoionization cross sections (PICSs) for quantification of measured mole fractions in OCM catalyzed by Li/MgO.

m/z	Species	Ionization energy (eV)	PICS	
			Value (Mb)	Ref.
15.03	CH_3 (methyl)	9.84	4.33 (11.5 eV)	[1]
16.03	CH_4 (methane)	12.61	Standard gas experiment	-
18.01	H_2O (water)	12.62	12.39 (14.5 eV)	[2]
26.04	C_2H_2 (acetylene)	11.40	Standard gas experiment	-
27.99	CO (carbon monoxide)	14.01	Standard gas experiment	-
28.03	C_2H_4 (ethylene)	10.51	Standard gas experiment	-
29.04	C_2H_5 (ethyl radical)	8.12	5.37 (11.5 eV)	[3]
30.01	CH_2O (formaldehyde)	10.88	38 (13 eV)	est
30.05	C_2H_6 (ethane)	11.52	Standard gas experiment	-
31.99	O_2 (oxygen)	12.07	Standard gas experiment	-
42.04	CH_2CO (ketene)	9.62	13 (11.5 eV)	est
42.05	C_3H_6 (propene)	9.73	13.35 (11.5 eV)	[4]
44.01	CO_2 (carbon dioxide)	13.78	Standard gas experiment	-
44.10	C_3H_8 (propane)	10.94	11.46 (11.5 eV)	[5]

Table S2. Estimates for the catalyst descriptors of Li/MgO catalyst for OCM.

	Catalyst descriptor	Unit	Value
D_1	Chemisorption enthalpy of O_2	kJ/mol	111
D_2	Reaction enthalpy of hydrogen abstraction of CH_4	kJ/mol	61
D_3	Chemisorption enthalpy of CO_2	kJ/mol	87
D_4	Chemisorption enthalpy of H_2O	kJ/mol	54
D_5	Density of active sites	mol/cm^2	2.25×10^{-10}

X-ray diffraction (XRD) spectrum

The XRD patterns did not detect any oxidation phase of Li, aligning with the findings of Qian et al.[6] This indicates that the calculated 5.6% Li loading primarily contributes to the structure modification of the MgO catalyst, consistent with previous conclusions[7-10] and the modeling hypothesis presented in this paper.

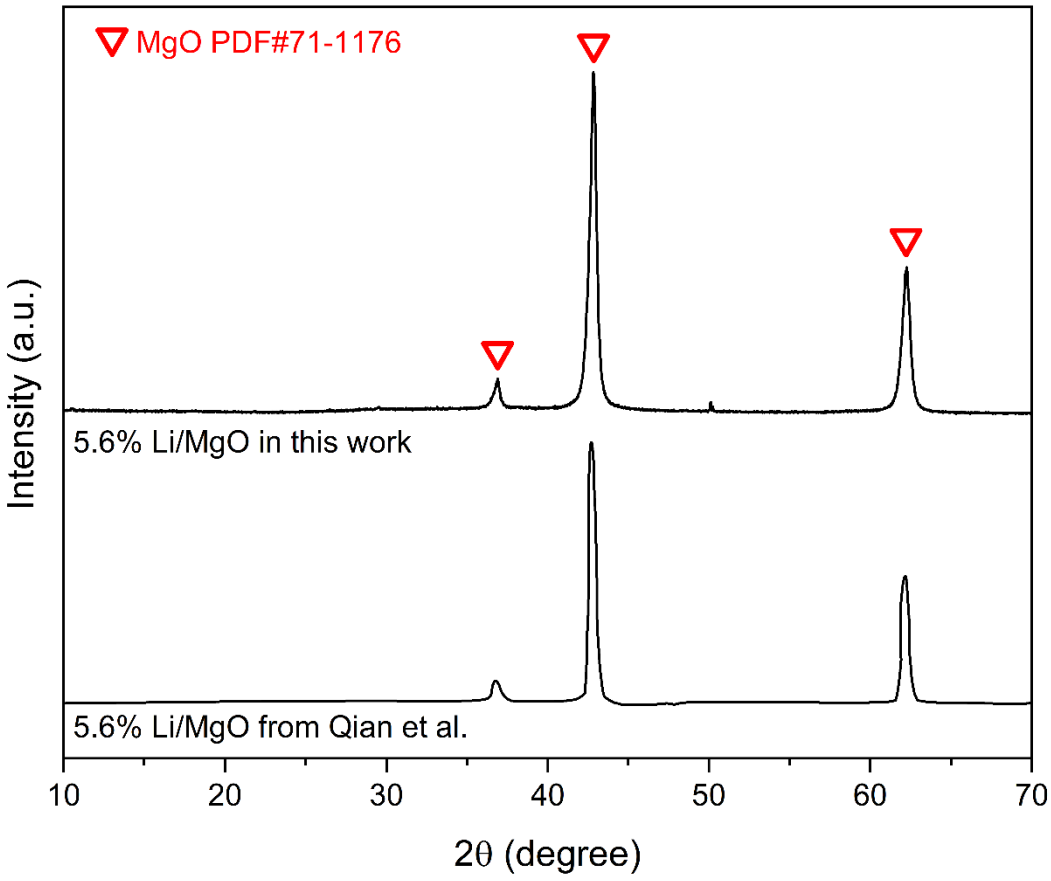

Figure S1. XRD patterns of Li-MgO catalysts with 5.6% calculated Li loadings.

References

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