

Supporting Information

Unraveling the role of particle size of active metal for Ni/MgO on methane activation and carbon growth mechanism

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Table S1 Frequency of CH_x on the Ni_x/MgO

Ni13/MgO	CH ₄ →CH ₃ +H	CH ₃ →CH ₂ +H	CH ₂ →CH+H	CH→C+H
Frequency (1/cm)	-523.13	-938.82	-665.88	-1010.97
	65.22	142.50	234.48	274.65
	222.04	214.51	285.41	294.62
	254.41	377.58	287.18	355.65
	331.27	413.35	459.07	426.78
	526.52	496.73	507.47	1148.26
	550.89	656.58	725.94	
	861.05	800.38	1455.67	
	972.47	1215.82	2958.81	
	1041.17	1290.25		
	1319.66	2852.87		
	1324.99	2956.31		
	2892.64			
	3006.18			
	3021.60			

Ni25/MgO	CH ₄ →CH ₃ +H	CH ₃ →CH ₂ +H	CH ₂ →CH+H	CH→C+H
Frequency (1/cm)	-356.82	-825.02	-967.94	-723.34
	24.18	119.29	225.05	101.52
	35.38	199.42	262.18	245.97
	141.49	308.01	307.71	361.47
	183.87	355.67	440.61	403.14
	332.61	488.71	527.99	818.86
	358.96	633.40	662.78	
	568.21	735.73	1,144.69	
	922.15	1,259.71	2,943.94	
	1,046.71	1,300.61		
	1,298.02	2,736.47		
	1,313.58	2,871.46		
	2,990.77			
	3,166.76			
	3,206.05			

Ni37/MgO	CH ₄ →CH ₃ +H	CH ₃ →CH ₂ +H	CH ₂ →CH+H	CH→C+H
Frequency (1/cm)	-308.71	-1022.68	-1066.86	-840.84
	25.63	102.58	157.29	271.30

	36.13	109.74	347.15	325.58
	124.54	268.45	415.17	357.99
	103.97	391.33	456.27	403.54
	213.88	480.52	486.57	1068.72
	257.79	583.34	642.34	
	462.92	704.93	1050.89	
	652.20	1199.90	2952.30	
	1160.86	1400.64		
	1257.82	2878.43		
	1290.13	3031.73		
	3030.65			
	3210.86			
	3253.92			