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Ni 掺杂对 Ni/MgO 体系中电荷分配影响

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Effect of Ni Doping on Electron Transfer in Ni/MgO Catalysts

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表 S1 Ni8/Ni_xMg_yO₂₇(1 0 0)上 CH₄/CO₂重整过程的反应物、中间体、产物的吸附能

Table S1 Adsorption energies of reactants, intermediates, and products in CH₄/CO₂ reforming on Ni8/Ni_xMg_yO(1 0 0).

Species	E _{ads} /eV			
	Cat-0	Cat-1	Cat-13	Cat-14
1 CH ₄ (p)	0.05	0.01	0.13	0.07
2 CH ₃ +H	-2.26	-2.27	-2.49	-2.13
3 CH ₃	-1.96	-1.97	-2.09	-1.75
4 CH ₂ +H	-4.13	-4.11	-4.40	-4.49
5 CH ₂	-3.97	-3.99	-3.68	-3.65
6 CH+H	-6.47	-6.71	-6.19	-5.97
7 CH	-6.84	-6.85	-5.87	-5.82
8 C +H	-8.12	-8.45	-7.74	-7.49
9 C	-7.57	-8.24	-7.35	-7.57
10 H	-0.40	-0.15	-0.36	-0.17
11 CO ₂ (p)	-0.05	-0.10	-0.08	-0.09
12 CO ₂	-0.57	-0.50	-0.30	-0.19
13 CO+O	-4.36	-4.32	-4.97	-4.69
14 CO	-1.81	-1.63	-1.67	-1.96
15 O	-2.83	-2.75	-3.39	-3.25
16 CH ₂ +O	-7.48	-6.99	-	-
17 CH ₂ O	-1.32	-1.04	-	-
18 CHO+H	-2.12	-2.22	-	-
19 CH+O	-	-	-9.30	-9.04
20 CHO	-2.58	-2.28	-2.33	-2.14
21 CO+H	-2.01	-1.93	-2.08	-2.01

表 S2 Ni8/Ni_xMg_yO₂₇(1 0 0)上 CH₄/CO₂重整过程最优反应路径的反应能垒和反应能

Table S2 Energetics of the most favored elementary steps in CH₄/CO₂ reforming on Ni8/Ni_xMg_yO₂₇(1 0 0).

Reactions	TS	Cat-0		Cat-1		Cat-13		Cat-14	
		E _B /eV	ΔH/eV	E _B /eV	ΔH/eV	E _B /eV	ΔH/eV	E _B /eV	ΔH/eV
1 CH ₄ (p) → CH ₃ + H	TS-1	2.24	0.12	2.34	0.15	2.70	-0.20	2.87	0.23
2 CH ₃ → CH ₂ + H	TS-2	1.54	0.86	1.33	0.89	2.68	0.72	2.63	0.23
3 CH ₂ → CH+H	TS-3	1.58	-0.31	1.92	-0.53	2.21	-0.32	1.93	0.05
4 CH → C + H	TS-4	1.13	0.89	1.68	0.87	1.99	0.60	2.21	0.84
5 CO ₂ (p) → CO ₂	TS-5	0.30	-0.52	0.09	-0.40	0.17	-0.22	0.65	-0.28
6 CO ₂ → CO + O	TS-6	1.45	0.14	1.75	0.11	1.15	-0.74	1.26	-0.57
7 CH ₂ + O → CH ₂ O	TS-7	2.40	0.05	2.20	-0.16	-	-	-	-
8 CH ₂ O → CHO + H	TS-8	1.65	0.89	1.96	0.51	-	-	-	-
9 CH + O → CHO	TS-9	-	-	-	-	2.48	0.36	2.58	0.29
10 CHO → CO +H	TS-10	0.34	-0.44	1.51	-0.66	1.20	-0.76	1.14	-0.98

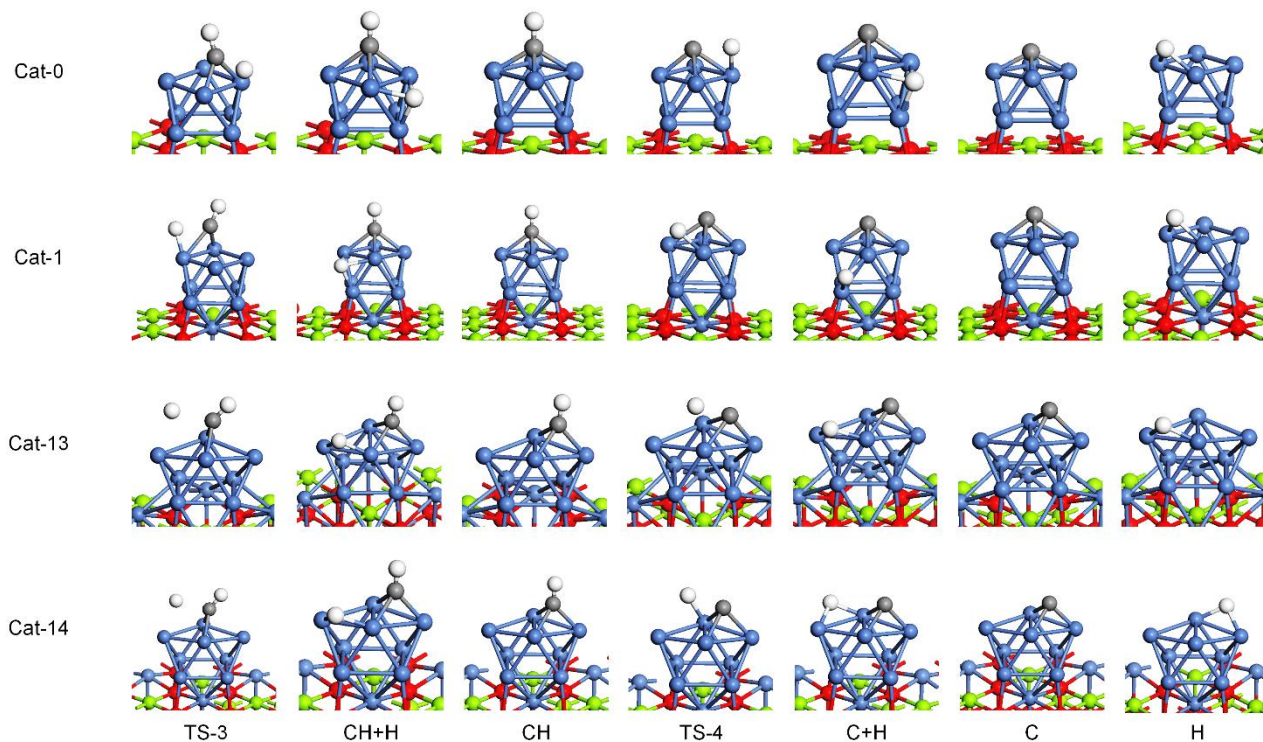
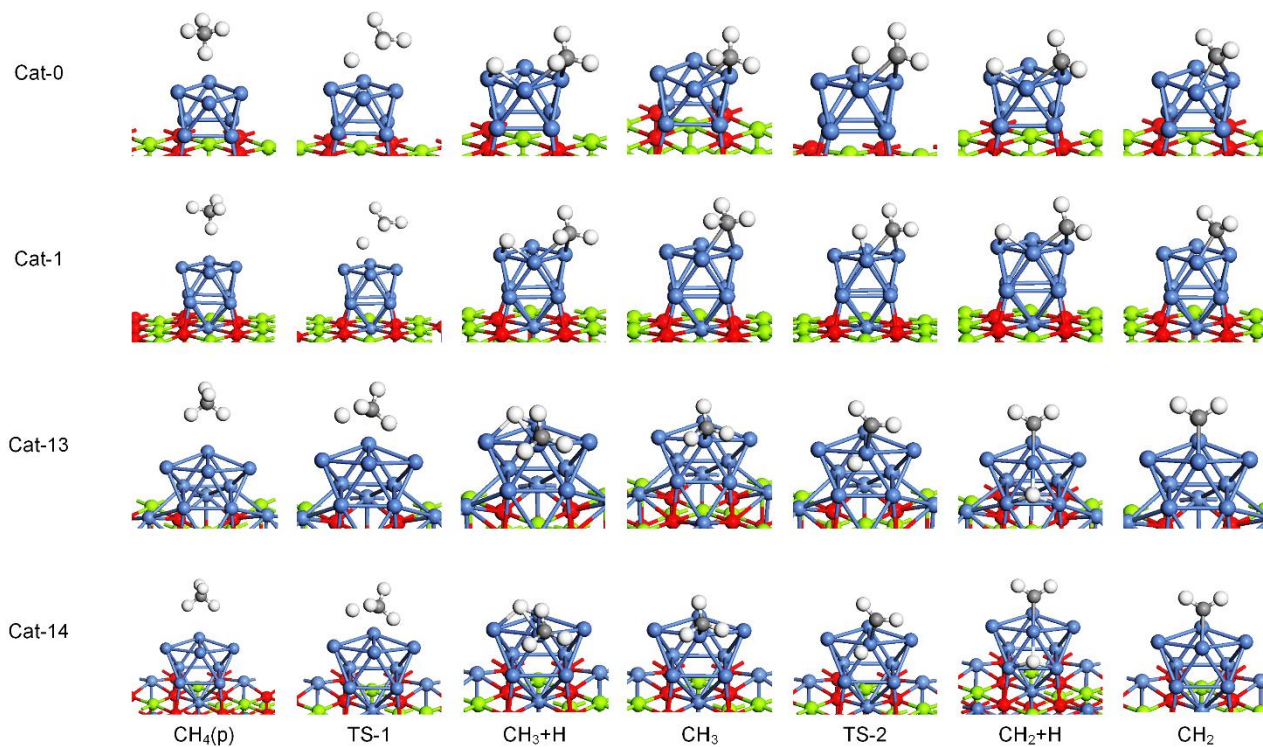


图 S1 Ni₈/Ni_xMg_yO₂₇(1 0 0)上 CH₄裂解过程中间体和过渡态的几何构型

Fig.S1 Geometries of adsorption configurations and transition structures in CH₄ dissociation on Ni₈/Ni_xMg_yO₂₇(1 0 0).

Color coding: Red, O atoms; Green, Mg atoms; Blue, Ni atoms; Grey, C atoms; White, H atoms

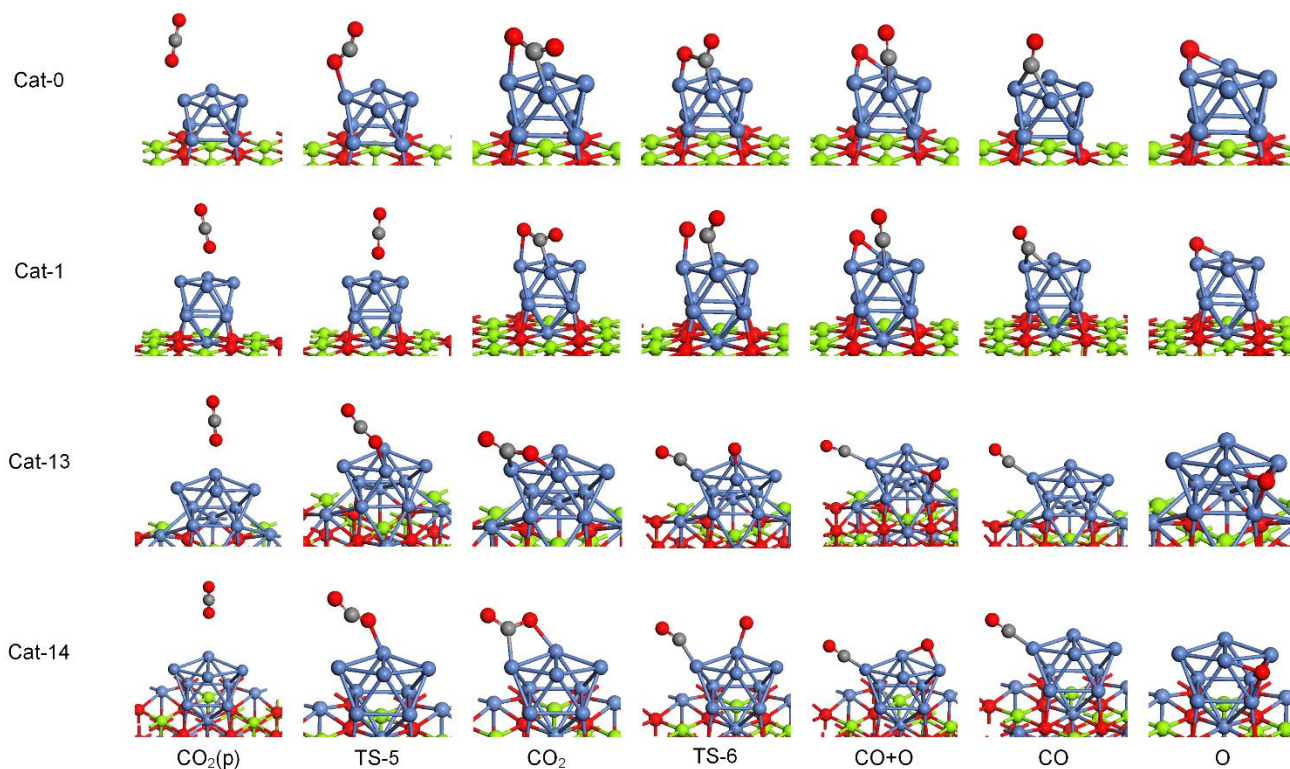


图 S2 Ni₈/Ni_xMg_yO₂₇(100)上 CO₂ 吸附解离过程中间体和过渡态的几何构型
Fig.S2 Geometries of adsorption configurations and transition structures in CO₂ adsorption and decomposition on Ni₈/Ni_xMg_yO₂₇(100).

Color coding: Red, O atoms; Green, Mg atoms; Blue, Ni atoms; Grey, C atoms; White, H atoms

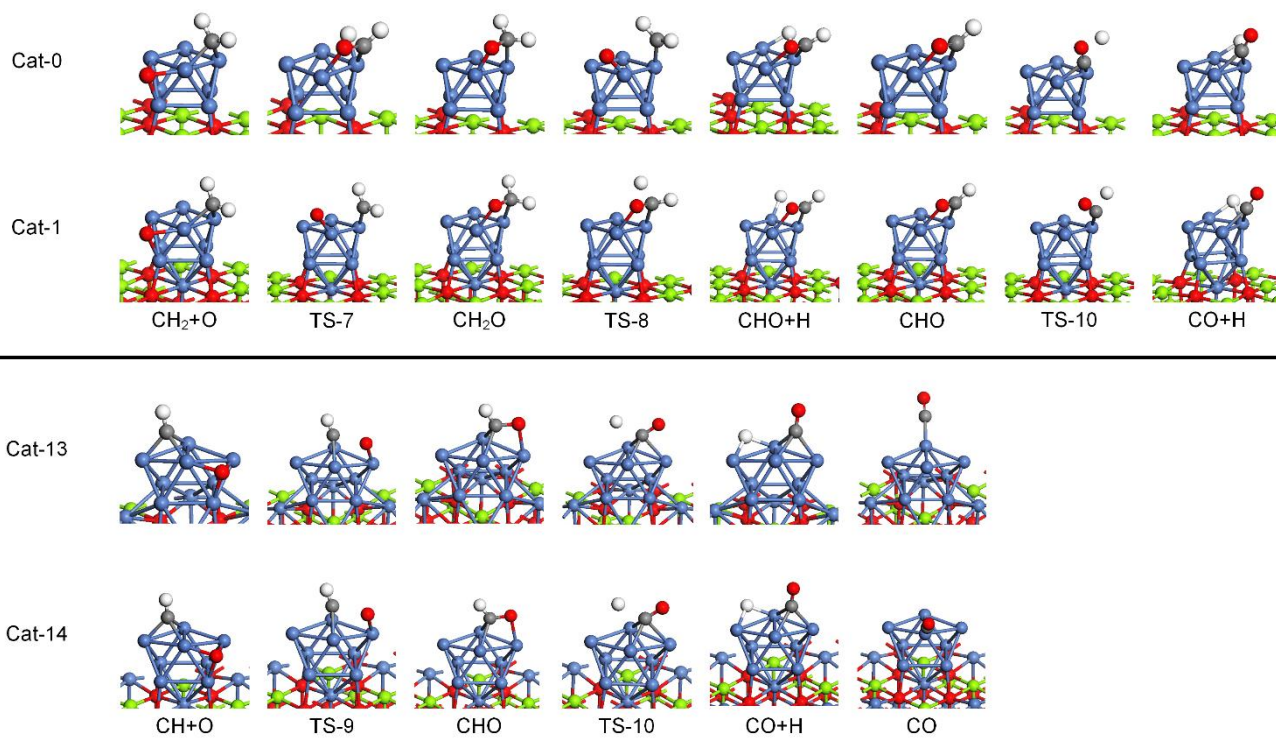


图 S3 $\text{Ni}_8/\text{Ni}_x\text{Mg}_y\text{O}_{27}(100)$ 上 CH_xO 生成与脱氢过程的中间体和过渡态的几何构型

Fig.S3 Geometries of adsorption configurations and transition structures in CH_xO formation and dehydrogenation on $\text{Ni}_8/\text{Ni}_x\text{Mg}_y\text{O}_{27}(100)$.

Color coding: Red, O atoms; Green, Mg atoms; Blue, Ni atoms; Grey, C atoms; White, H atoms