Electronic Supplementary Material

A density functional theory study of methane activation on MgO supported Ni_9M_1 cluster: Role of M on C–H activation

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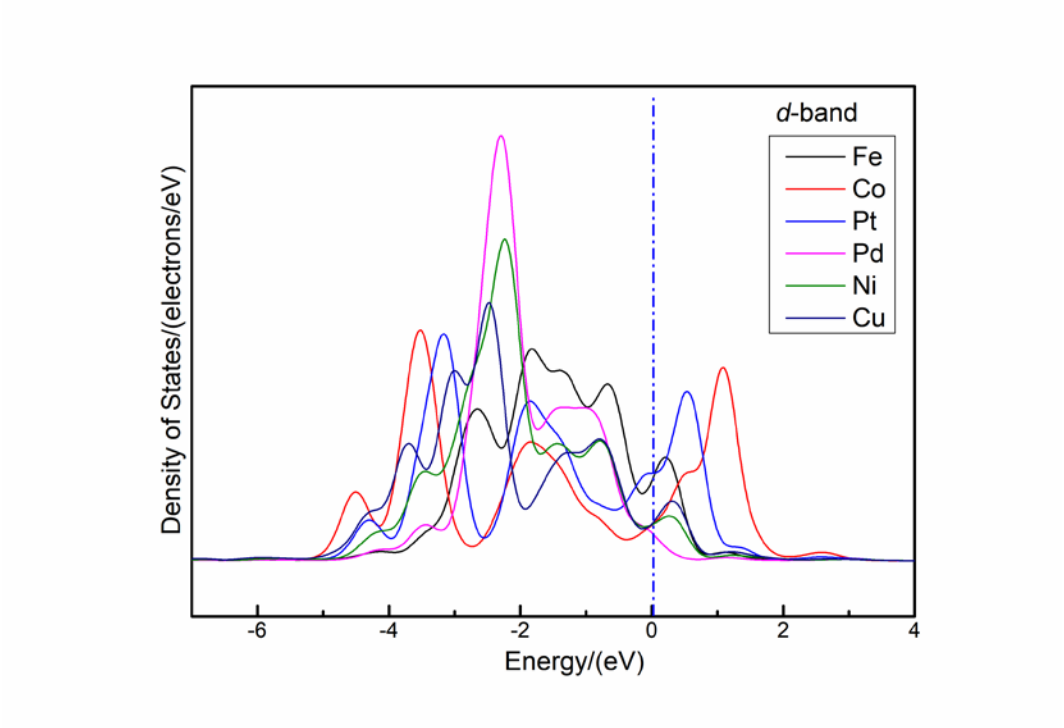

Figure S1 Density of states of *d*-band for doping atom M in the isolated catalysts. The blue dash line represents the Fermi level.

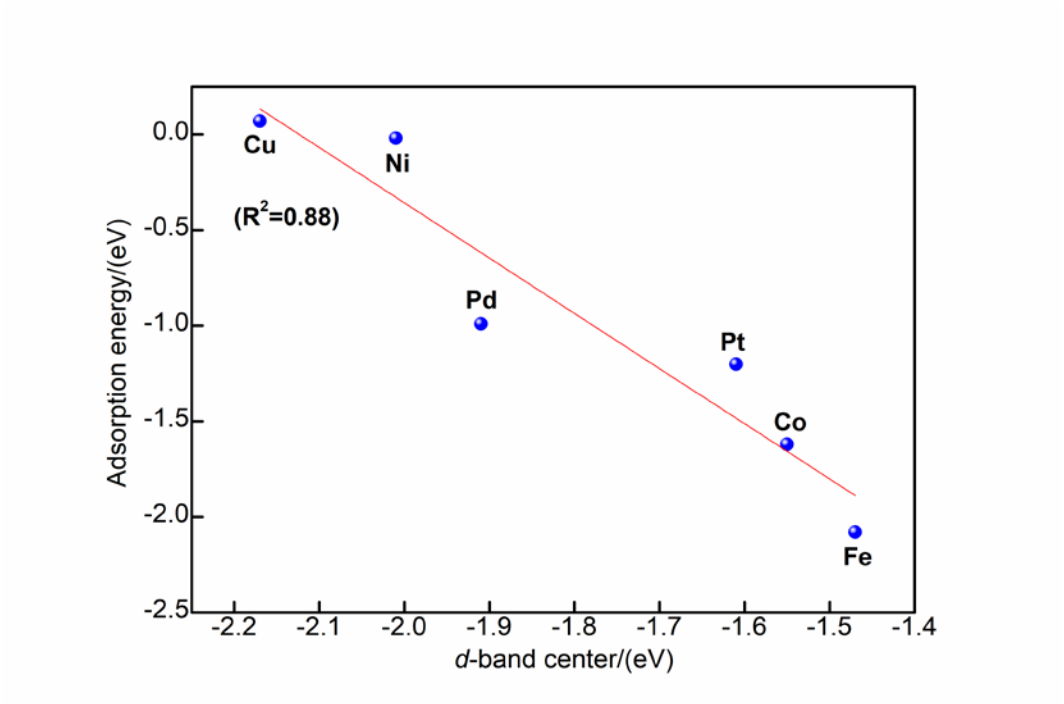

Figure S2 The relationship between *d*-band center of doping atom M and adsorption energy of CH_4 molecule.

Table S1 Energies of the IS, TS and FS states for each catalyst (eV).

	Ni	**Fe**	**Co**	**Cu**	**Pd**	**Pt**
CH_4(g)+ Catalysts (isolated)	-104221.88	-103730.59	-103908.74	-104346.15	-103665.58	-103586.76
IS(CH_4 ads)	-104221.90	-103732.67	-103910.36	-104346.08	-103666.57	-103587.96
TS(CH_3--H)	-104221.35	-103732.26	-103909.74	-104344.84	-103665.63	-103587.17
FS(CH_3+H)	-104222.03	-103732.94	-103910.48	-104345.31	-103666.25	-103587.90

Table S2 Mulliken atomic charges (e) for every element in Ni_9M_1 clusters.

	M	Ni1	Ni2	Ni3	Ni4	Ni5	Ni6	Ni7	Ni8	Ni9	Total
Fe	0.07	-0.24	-0.23	-0.23	-0.23	0.03	0.03	0.04	0.03	-0.47	-1.47
Co	0.02	-0.24	-0.23	-0.24	-0.23	0.05	0.05	0.05	0.05	-0.46	-1.18
Ni	-0.13	-0.22	-0.22	-0.22	0.03	0.04	0.03	0.03	-0.41	-0.04	-1.11
Cu	-0.16	-0.24	-0.24	-0.24	-0.23	0.07	0.08	0.07	0.07	-0.25	-1.07
Pd	-0.37	-0.24	-0.24	-0.24	-0.23	0.13	0.13	0.13	0.13	-0.38	-1.18
Pt	-0.41	-0.23	-0.22	-0.23	-0.22	0.13	0.13	0.13	0.11	-0.43	-1.24