

Table S1 The adsorption energy (E_{ads} , eV), bond length between Fe and CH_x ($d_{\text{Fe-CH}_x}$, Å), transferred electrons from the substrates to the CH_x (Δq_{CH_x} , e), and total magnetic moment (m , μ_{B}) for the adsorbed CH_x ($x=0\sim 4$) on the Fe-graphene systems (including the top site of metal atom and metal-carbon bond).

Systems		Fe-graphene		
CH_x species	E_{ads} (eV)	$d_{\text{Fe-CH}_x}$ (Å)	Δq_{CH_x} (e)	M (μ_{B})
C	3.42	1.72	+0.48	1.70
	4.57	1.61	+0.47	0.00
CH	3.70	1.78	+0.47	1.00
	4.37	1.82	+0.40	3.00
CH_2	3.01	1.88	+0.43	2.00
	4.00	1.97	+0.24	2.00
CH_3	2.40	1.96	+0.40	1.00
	1.38	2.18	+0.22	1.00
CH_4	0.17	2.44	-0.03	0.00