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**Table S1** The adsorption energy ( $E_{ads}$ , eV), bond length between Fe and  $CH_x$  ( $d_{Fe\text{-}CHx}$ , Å), transferred electrons from the substrates to the  $CH_x$  ( $\triangle q_{CHx}$ , e), and total magnetic moment (m,  $\mu_B$ ) for the adsorbed  $CH_x$  ( $x=0\sim4$ ) on the Fe-graphene systems (including the top site of metal atom and metal-carbon bond).

Systems	Fe-graphene			
CH <sub>x</sub>	E <sub>ads</sub>	d <sub>Fe-CHx</sub>	$\triangle q_{CHx}$	M
species	(eV)	(Å)	(e)	$(\mu_{\mathrm{B}})$
C	3.42	1.72	+0.48	1.70
	4.57	1.61	+0.47	0.00
СН	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 <sub>3</sub>	2.40	1.96	+0.40	1.00
	1.38	2.18	+0.22	1.00
CH <sub>4</sub>	0.17	2.44	-0.03	0.00