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ARTICLE

Direct Oxidation of Methane to Methanol on Fe–O Modified Graphene

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Table S1. Atomic partial charges of the reaction intermediates along the singlet and triplet spin state reaction coordinates for the conversion of methane to methanol over the FeO/graphene catalyst. Values were obtained from the Hirshfeld population analysis. The values in parenthesis are for the triplet spin states.

Atom/Molecule	Charge (*e*)					
	Isolated state	**ADS**	**TS1**	**INT**	**TS2**	**PROD**
Fe	+0.190 (+0.208)	+0.196 (+0.214)	+0.157 (+0.193)	+0.175 (+0.196)	+0.137 (+0.192)	+0.141 (+0.202)
O	–0.259 (–0.265)	–0.244 (–0.249)	–0.125 (–0.246)	–0.271 (–0.290)	–0.186 (–0.232)	–0.091 (–0.116)
H	0.038	+0.028 (+0.027)	+0.091 (+0.052)			
C	-0.149	–0.165 (–0.165)	–0.158 (–0.101)			
Graphene	+0.071 (+0.060)	+0.084 (+0.073)	–0.103 (–0.042)	–0.056 (–0.066)	–0.230 (–0.182)	–0.426 (–0.408)
CH_4 molecule	0.000	–0.033 (–0.035)				
CH_3OH molecule	0.000					+0.288 (+0.209)
Methyl group			–0.018 (+0.044)	–0.014 (+0.048)	+0.125 (+0.079)	
Hydroxyl group				–0.131 (+0.176)	–0.029 (–0.087)	

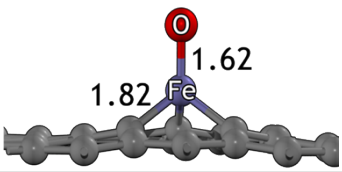
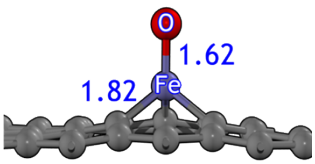
Structure	Singlet state	Triplet state
Isolated FeO/graphene		

Fig. S1. Optimized structure of the FeO/graphene calculated at the PBE level of theory.

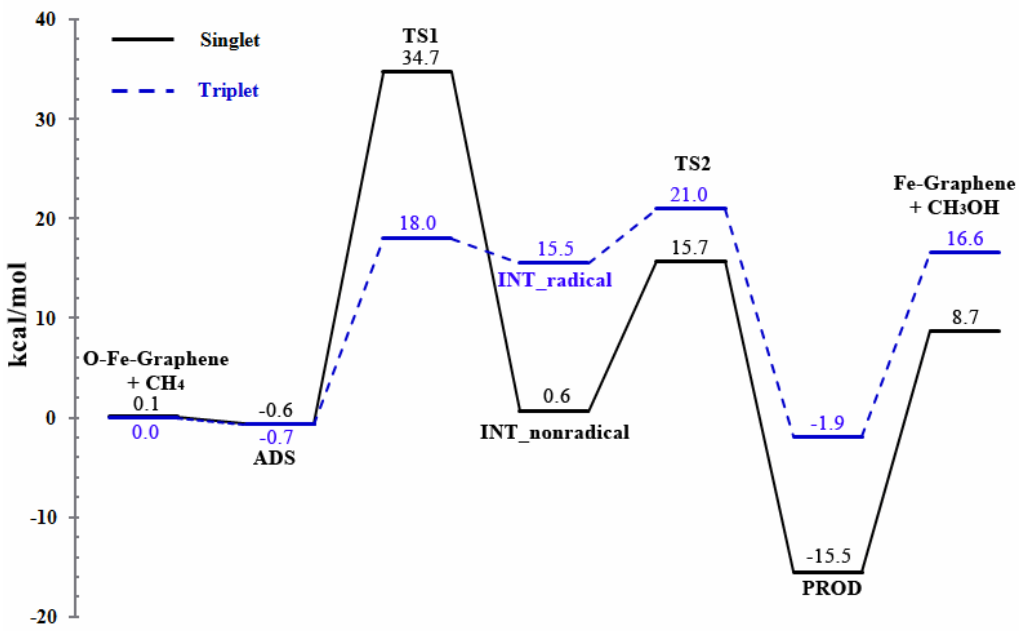


Fig. S2. Energy profile for the direct oxidation of methane to methanol over FeO/graphene calculated at the PBE level of theory.

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