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"Supporting Information"

Epoxidation of ethylene over Pt-, Pd- and Ni-doped graphene in the presence of N_2O as an oxidant: A comparative DFT study

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Figure S1. The energy diagram for the diffusion of M= Pt, Pd or Ni atom on the M-doped graphene sheet. The IS, TS and P represent initial structure, transition structure and final product, respectively.

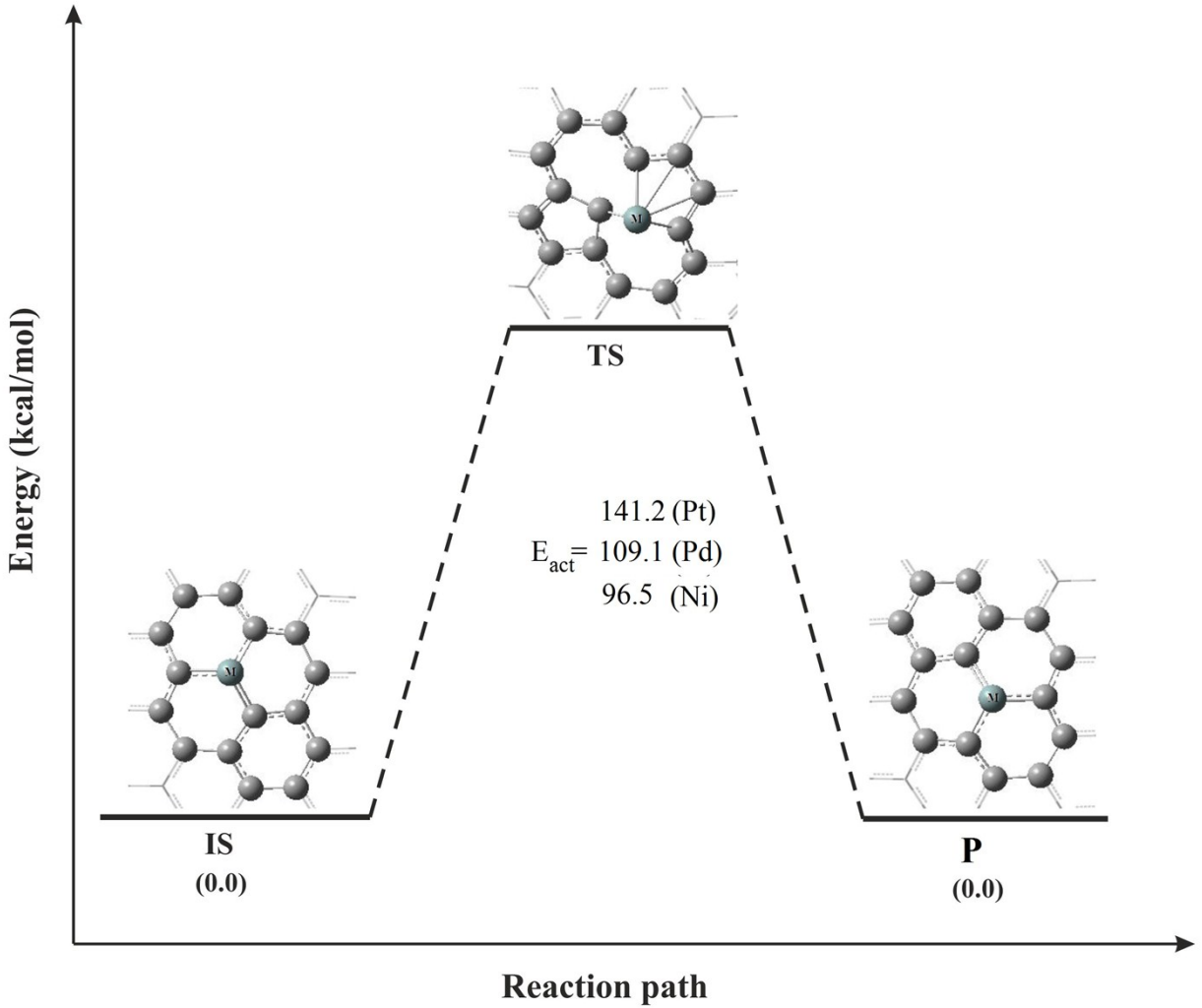

Figure S2. The large model used for the M-doped graphene (M=Ni, Pd and Pt)

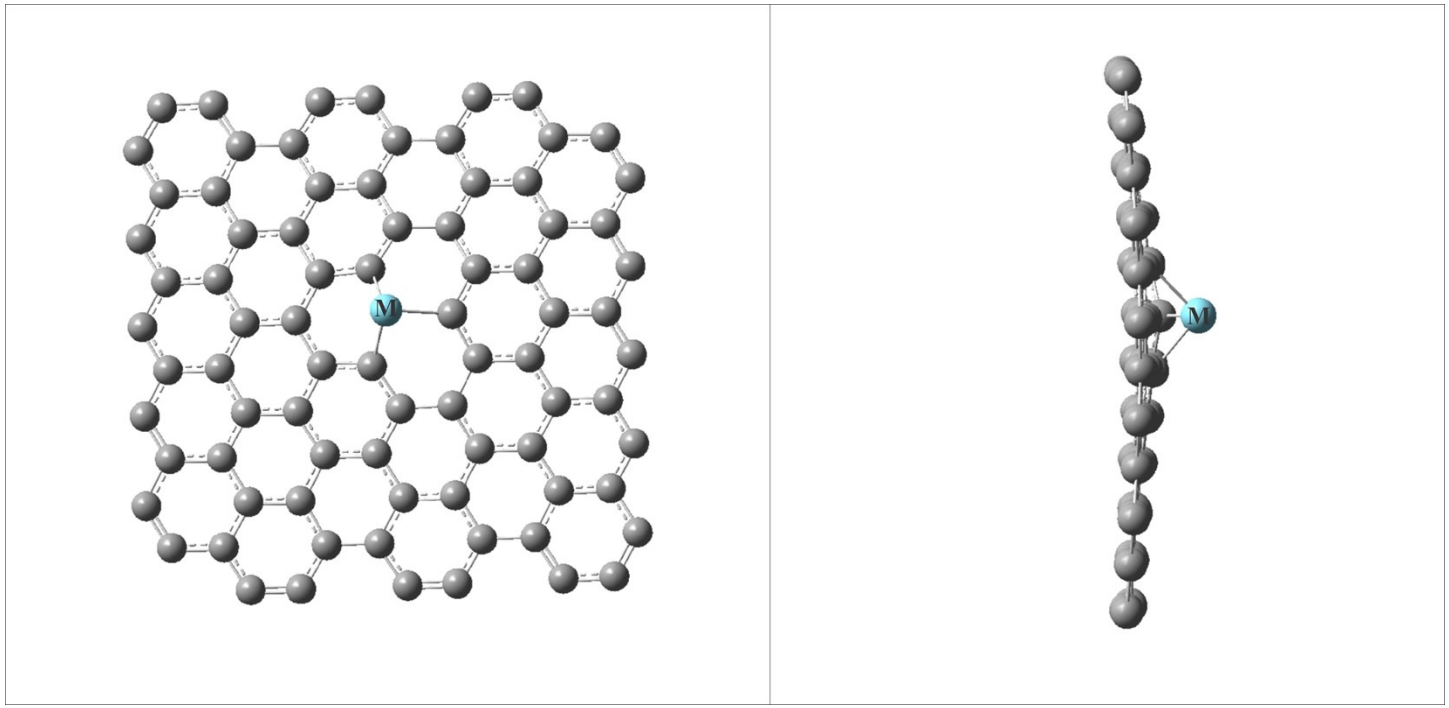

Table S1. Calculated (M06-2X/6-311+G*/LANL2DZ) adsorption energy (E_{ads}) for the adsorption/co-adsorption of N_2O and C_2H_4 molecules over Pt-/Pd-/Ni-G surfaces

Complex	E_{ads} (kcal mol^{-1})
Pt-G	
A	-15.1
B	-5.0
G	-25.3
Pd-G	
C	-10.1
D	-9.2
H	-19.7
Ni-G	
E	-7.5
F	-6.4
I	-16.5

Table S2. Calculated adsorption energy (E_{ads}) for the adsorption/co-adsorption of N_2O and C_2H_4 molecules over the large Pt-/Pd-/Ni-G model

Complex	E_{ads} (kcal mol^{-1})
Pt-G	
A	-15.5
B	-5.3
G	-26.1
Pd-G	
C	-10.6
D	-9.6
H	-20.3
Ni-G	
E	-8.0
F	-6.8
I	-16.9