

“Supporting Information”

Oxidation of CO by N₂O over Al- and Ti-doped graphene: A comparative study

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Figure S1. The energy profile for the diffusion of M=Al or Ti atom on the graphene. IS, TS and FS represent initial structure, transition structure and final structure, respectively.

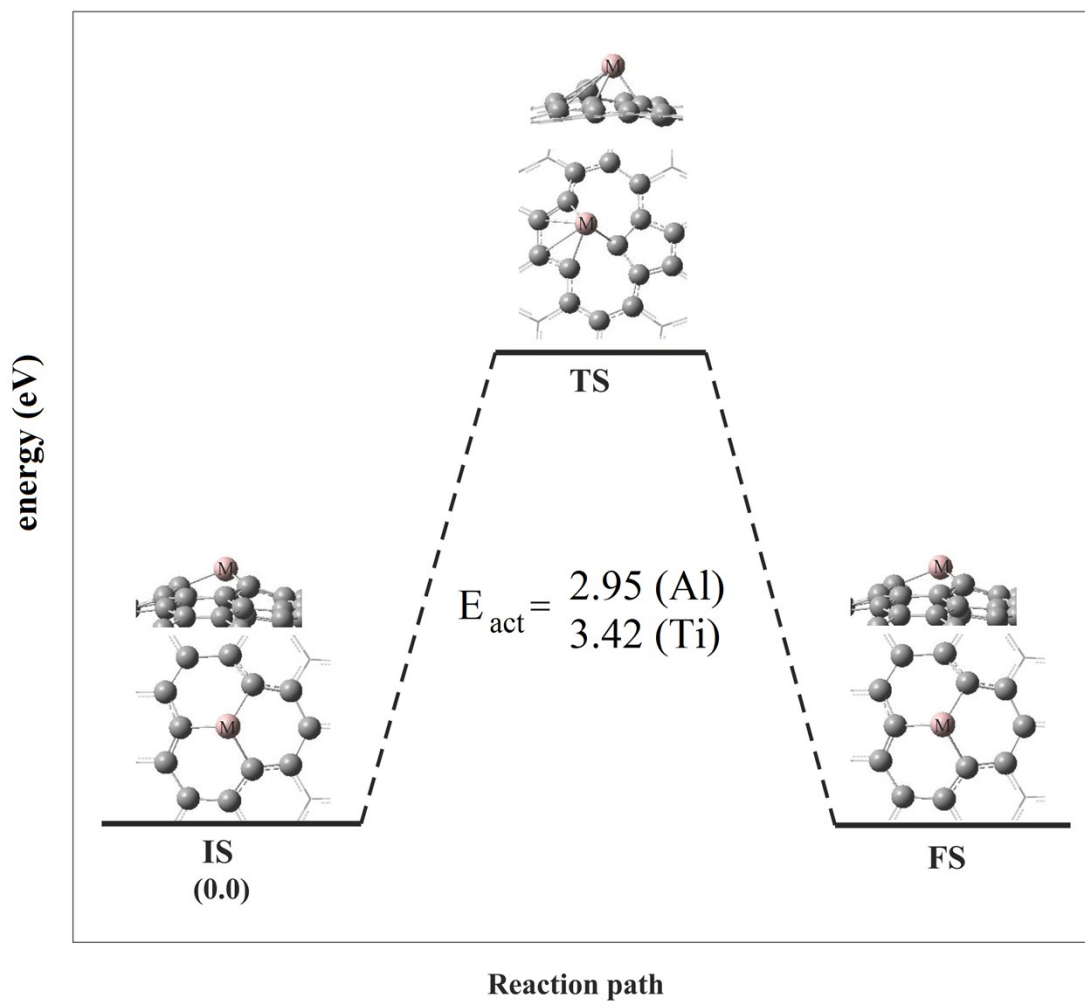
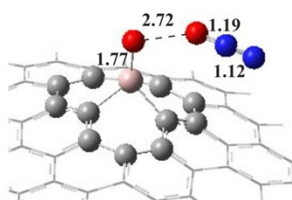


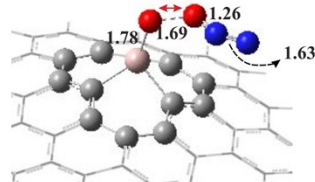
Figure S2. Schematic energy profile corresponding to local configurations along the $\text{O}_{\text{ads}} + \text{N}_2\text{O} \rightarrow \text{N}_2 + \text{O}_2$ reaction pathway over Al-/Ti-graphene sheet. All energies and bond distances are in eV and Å, respectively.

Al-graphene

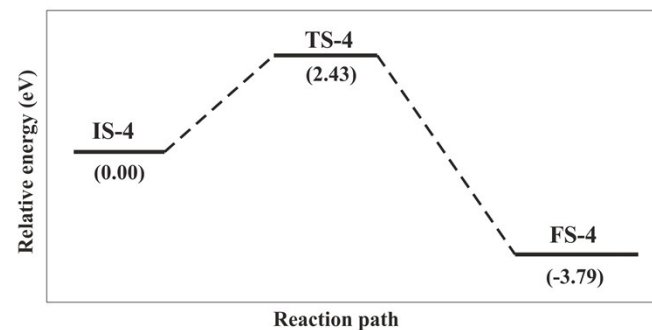
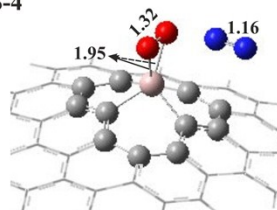
IS-4



TS-4

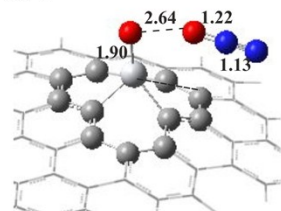


FS-4

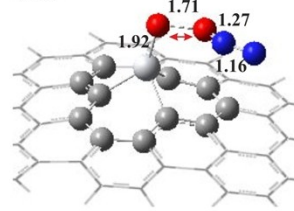


Ti-graphene

IS-5



TS-5



FS-5

