

## “Supplementary Materials”

### **Activation of the methane C-H bond by Al- and Ga-doped graphenes: A DFT investigation**

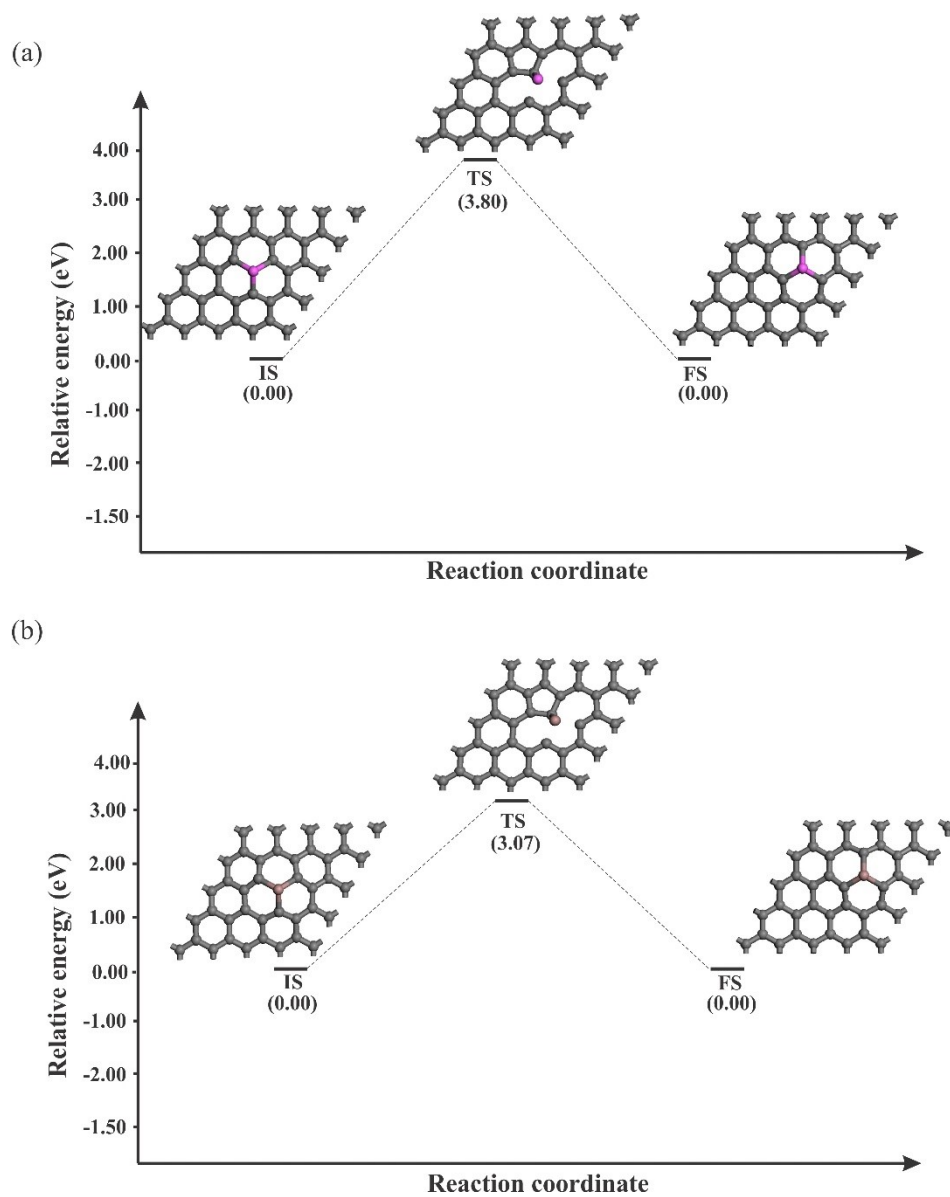
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**Figure S1.** Energy profile and activation barrier for diffusing the (a) Al and (b) Ga atom on graphene



**Figure S2.** The adsorption of CH<sub>4</sub> via the C-H bond on (a) Al-Gr and (b) Ge-Gr

