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# Methyl Radical Addition to the Surface of Graphene Nanoflakes: A Density Functional Theory Study

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**Highlights**

- Activation energies for the addition of methyl radical ($CH_3$) to a graphene surface were systematically determined by density functional theory method.
- Binding energies between $CH_3$ and the graphene surface were determined.
- Absorption and IR spectrum of methylated graphene were theoretically predicted.
- Hyperfine coupling constant of methylated graphene was theoretically predicted.

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