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# Computational Study of CO<sub>2</sub> Adsorption and Reduction on Doped Graphene Sheets

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## Computational Study of CO<sub>2</sub> Adsorption and Reduction on Doped Graphene Sheets

In recent decades, growing CO<sub>2</sub> in the Earth's atmosphere has become a major issue.

Thus, it is crucial to reduce the level of concentration of CO<sub>2</sub> in the atmosphere.

We have investigated the adsorption and reduction of CO<sub>2</sub> on metal-doped graphene sheets, through computational methods. The electrochemical reduction of CO<sub>2</sub> to CO, CH<sub>3</sub>OH and CH<sub>4</sub> were calculated. Co-doped graphene sheet shows very promising catalytic behavior for CO<sub>2</sub> reduction with the highest elemental reaction energy less than 0.7 eV. In addition, the reaction pathways reveal the possible rate limiting step could be the removal of the second H<sub>2</sub>O, CH<sub>3</sub>OH or CH<sub>4</sub> from the doped graphene sheet, depending upon the type of dopant in graphene.