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Computational Study of CO2 Adsorption and Reduction on Doped Graphene Sheets

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In recent decades, growing CO_2 in the Earth's atmosphere has become a major issue.

Thus, it is crucial to reduce the level of concentration of CO_2 in the atmosphere.

We have investigated the adsorption and reduction of CO_2 on metal-doped graphene sheets, through computational methods. The electrochemical reduction of CO_2 to CO, CH_3OH and CH_4 were calculated. Co-doped graphene sheet shows very promising catalytic behavior for CO_2 reduction with the highest elemental reaction energy less than 0.7 eV. In addition, tThe reaction pathways reveal the possible rate limiting step could be the removal of the second H_2O, CH_3OH or CH_4 from the doped graphene sheet, depending upon the type of dopant in graphene.