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Computational Study of CO₂ Adsorption and Reduction on Doped Graphene Sheets

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Computational Study of CO₂ Adsorption and Reduction on Doped Graphene Sheets

In recent decades, growing CO₂ in the Earth's atmosphere has become a major issue.

Thus, it is crucial to reduce the level of concentration of CO₂ in the atmosphere.

We have investigated the adsorption and reduction of CO₂ on metal-doped graphene sheets, through computational methods. The electrochemical reduction of CO₂ to CO, CH₃OH and CH₄ were calculated. Co-doped graphene sheet shows very promising catalytic behavior for CO₂ 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 H₂O, CH₃OH or CH₄ from the doped graphene sheet, depending upon the type of dopant in graphene.