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Molecular Simulation Study on the Catalytic Role of Silicon-Doped Graphene in Carbon Dioxide Hydrogenation

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Abstract : The theoretical investigation of Si-doped graphene nanoflakes (NFs) was conducted to understand their catalytic impact on CO_2 reduction using molecular hydrogen at the Density Functional Theory (DFT) level. The introduction of silicon by substituting carbon induces defects in the NF structure, resulting in a polyradical ground state. This silicon defect significantly boosts reactivity towards substrates, making Si-doped graphene NFs more catalytically active in CO_2 reduction to formic acid compared to silicene. Notably, Si-doped graphene demonstrates a preference for formic acid over carbon monoxide, mirroring the behavior of silicene. Furthermore, investigations into formic acid-to-formaldehyde and formaldehyde-to-methanol conversions reveal instances where Si-doped graphene outperforms silicene in terms of efficacy. In the final reduction step, the methanol-to-methane reaction unfolds in four stages, with the rate-determining step involving hydrogen transfer from silicon to methyl. Notably, the activation energy for this step is lower in Si-doped graphene compared to silicene. Consequently, Si-doped graphene NFs emerge as superior catalysts with lower activation energies overall. Remarkably, throughout these catalytic processes, Si-doped graphene maintains environmental stability, further highlighting its enhanced catalytic activity without compromising graphene's inherent stability.

Keywords : silicon-doped graphene, CO_2 reduction, DFT, catalysis
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