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First-principles study of H₂ adsorption on two-dimensional C₂N sheet

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First-principles calculations based on density functional theory (DFT) have been performed to study the adsorption of molecular H₂ on the graphene-like material C₂N. The possible adsorption sites on top of bonds, on carbon atom and nitrogen atom and the center of C-C hexagon and the C-N hexagon are considered. The adsorption energies for each site are calculated and are found to be in the physisorption regime. We find that the most favorable site of H₂ is above the center of C-N hexagon. In addition, we demonstrate that inclusion of the Van der Waals interactions through the DFT-D2 method via the generalized gradient approximation (GGA) functional gives the consistent trend of H₂ adsorption with that obtained via the local-density approximation (LDA) functional. The effects of Van der Waals interactions on the adsorption energies and equilibrium distance between H₂ and C₂N sheet are discussed.

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