DFT study of Ti-decorated C_5N monolayer for High-performance Hydrogen Storage

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Hydrogen energy is a promising renewable energy source with the potential to replace fossil fuels, particularly for fuel cell vehicles (FCVs). However, efficient hydrogen storage remains a significant challenge for practical applications. In this study, we investigate the hydrogen storage properties of a nanoporous penta-carbon nitride (C_5N) material using spin-polarized density functional theory (DFT) calculations with van der Waals corrections. To enhance hydrogen adsorption properties, C_5N was decorated with Ti, which significantly improved its hydrogen storage capabilities. In addition, the decoration of transition metals on C_5N exhibits strong binding energies of -4.02 eV, attributed to charge transfer from the metal atoms to the pristine C_5N surface. Additionally, high diffusion barriers effectively prevent metal clustering, ensuring uniform dispersion and structural stability. To optimize hydrogen storage capacity, we systematically investigated configurations with up to six transition metal atoms placed on stable equivalent sites. The results reveal that each transition metal atom adsorbs up to six H_2 molecules -0.283 eV/H_2 for 6Ti@C_5N. These configurations achieve a gravimetric capacity of 5.73 wt%, meeting the U.S. Department of Energy (DOE) targets. A detailed electronic structure analysis indicates that the enhanced hydrogen storage capability of transition metal-decorated C_5N arises from a combination of polarization effects and the induced Kubas-type interaction. Furthermore, charge density difference and Bader charge analyses confirm strong interactions between hydrogen molecules and transition metals. These findings suggest that transition metal-decorated C_5N is a promising candidate for high-performance hydrogen storage applications, paving the way for advancements in hydrogen-based energy solutions.