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Theoretical investigation of carbon nitride nanothreads and polymer nanocomposites

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Abstract: Incorporating nanoscale reinforcements into polymer matrices offers an effective way to enhance the multifunctional performance of polymer nanocomposites. Carbon-based nanomaterials (CNMs) are widely explored for this purpose because of their exceptional strength, stability, and large interfacial surface area that enable efficient stress transfer. Among them, diamond nanothreads (DNTs) have attracted attention for their one-dimensional sp^3-bonded framework and hydrogen-terminated surfaces, which impart remarkable tensile strength, stiffness, and torsional resistance. Extending this concept, carbon nitride nanothreads (CNNTHs) have emerged as new candidates. The incorporation of nitrogen atoms enhances their structural versatility and narrows their electronic band gaps, making them attractive for designing polymer nanocomposites that combine robust mechanical properties with tunable electronic properties. This study employs first-principles simulations to explore the interfacial interactions and electronic properties of CNNTH/polymer nanocomposites. Cellulose and epoxy matrices were modeled in various orientations relative to CNNTHs. Charge Density Difference (CDD) and Electron Localization Function (ELF) analyses revealed charge redistribution primarily along the interface, with no ELF overlap, indicating interactions dominated by van der Waals forces. Electronic structure calculations further showed a 1 eV reduction in band gap compared to DNT/polymer systems. These results demonstrate CNNTHs'potential as reinforcements for high-performance polymer nanocomposites in advanced structural systems and flexible electronics.

Key Words: polymer; CNNTH; nanocomposites; electronic properties

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