Heteroatom-Doped Graphdiyne Enables Ferromagnetism of Carbon

A known doping atomic-level functionalization strategy achieves the breakthrough of ferromagnetism in carbon.

The rise and prosperity of graphdiyne have enriched the family of carbon materials. As a carbon semiconductor material, its direct band gap, highly conjugated structure, and impressive intrinsic mobility are attractive features that give potential to various applications such as energy conversion and storage and spin transistors. The rapid development and broad application of graphdiyne materials have driven the exploration of its intrinsic properties and of regulating methods for its functional integration. Li and co-workers have developed an atomic-level functionalization strategy to introduce different light elements into graphdiyne to achieve a ferromagnetic semiconductor.

Li and colleagues have used the new theories and knowledge of interdisciplinary science in graphdiyne-related research and revealed the key role of heteroatom doping in physical performance optimization and device promotion.

This work, like the construction of a pyramid (as shown in Figure 1a), is indispensable and precisely establishes the relationship between chemical doping and physical property control. It provides the fundamental understanding of graphdiyne’s ferromagnetic origin.

For semiconductor materials, the realization of the dual regulation of spin and charge for promoting the directional performance in the fields of semiconductor and information technology has always been a critical issue. The graphdiyne semiconductor, accompanied by its inherent band gap, could be useful in the preparation of new ferromagnetic semiconductors. In recent years, the research on the magnetic properties of graphdiyne show that it is a promising candidate for carbon-based spintronics and will attract intensive interest in this field. Generally, doping as a defect engineering strategy can effectively regulate the physical properties of materials and optimize the optical, electrical, magnetic, and other macroproperties as well as local properties. Thus, it is critical to reveal the role of chemical modification in tuning graphdiyne’s physical properties, which may contribute to the functionalization of such a carbon material.

Li and colleagues have used the new theories and knowledge of interdisciplinary science in graphdiyne-related research and revealed the key role of heteroatom doping in physical performance optimization and device promotion. Inductive local magnetic moment and its interaction are considered to be effective means to realize long-range ferromagnetic order and expand the application of materials in electronic devices.

In the latest report, Li and co-workers utilized bottom-up molecular design strategies to achieve precise modification.
of heteroatoms in graphdiyne materials. They investigated the effects of different types of elements such as Cl, H, and F on the magnetic properties. The self-assembled strategy provides a convenient and accurate route to doping different functional atoms at specific sites in graphdiyne semiconductors. In a series of graphdiyne-based materials, fluorine doping on their benzene rings not only demonstrated unique ferromagnetism and excellent mobility value but also an impressive performance in the materials when it was incorporated into the prototype of flexible electronic devices as shown in Figure 1. The strong ferromagnetic order of FsGDY at low temperatures indicates the interaction between the induced local magnetic moments. Interestingly, the mobility of this material can reach 320 cm² V⁻¹ s⁻¹ and be used to construct flexible FET devices, suggesting the enhanced charge migration characteristics resulting from the introduction of the fluorine element, which are further clarified by DFT calculations. Unlike H or Cl doping, fluorine doping leads to remarkable charge transfer, which promotes the exchange of local magnetic moments to induce ferromagnetism. If atoms with different electronegativity can be selected for doping, it will undoubtedly lead to precise tuning of the physical properties of graphdiyne. Beyond doping, the recent study suggests that the topological defects in diverse carbon species can also give rise to nondoubly degenerate states of both the π and π* bands near Fermi level (E_F), leading to tunable conductivity. Overall, these results provide methodological support for future work and contribute to targeted performance modulation.

Aiming at the next generation of carbon-based electronic devices, the research on the modification of advanced carbon materials such as graphdiyne and graphene will continue to be of interest as such studies can provide a reference for the breakthrough of new materials and new physical properties. The work of Li et al. strongly suggests the role of precise doping in the modification of targeted carbon materials. It offers a promising opportunity for the application of carbon semiconductors in electronic information technology.

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