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Electronic properties of doped graphene nanomesh structures using density functional theory

By

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Summary

In this study, we used first-principles density functional theory (DFT) calculationsto investigate the creation (induction) of magnetic moments in graphene nanomesh (GNM) monolayer sheets through substitutional doping with 3d transition metal atoms (M = Sc, Ti, V, Mn, Co, Ni, Cu, Zn). Our investigation focuses on three passivated systems: hydrogen-passivated GNM (H-GNM), nitrogen-passivated GNM (N-GNM), and oxygen-passivated GNM (O-GNM).

- Structural Implications:

  H-GNM: Substitutional doping in H-GNM preserves the planar geometry of the pristine graphene sheet. This implies that hydrogen passivation allows theGNM to maintain its plane structure despite the introduction of metal atoms.

  N-GNM and O-GNM: In contrast, doping in M-N-GNM and M-O-GNM systems causes the metal atoms to protrude from the GNM plane. This structural deviation indicates a more significant interaction between the dopant atoms and the nitrogen or oxygen-passivated GNMs, leading to a three-dimensional displacement.

- Stability Analysis:

  The study reveals that TM-N-GNM and TM-O-GNM systems are more stable than TM-H-GNM systems. This suggests that nitrogen and oxygen passivation have greater stability to the doped GNMs compared to hydrogen passivation. Among the different metal dopants, cobalt (Co) in H-GNM and titanium (Ti) in N-GNM and O-GNM exhibit the most stable structures. Zinc (Zn) demonstrates the highest formation energy across all three configurations, indicating that it is less favorable for doping in GNMs.

- Electronic and Magnetic Properties:

  Doping induces significant changes in the electronic structure of the GNMs, leading to the creation of new states around the Fermi energy. This alteration reduces the energy gaps in all systems compared to their pristine systems. Some doped systems transition from semiconductors to P-type semiconductors or diluted magnetic semiconductors (DMSCs). This transformation opens up potential applications in spintronics and electronic devices.

- Influence of Dopant Position:

  The position of the metal atom within the GNM supercell significantly affects the electronic and magnetic properties of the material. In several cases, the magnetization and energy gap values vary based on the dopant's placement. For instance, magnetic moments are observed only at specific positions in certain configurations, highlighting the critical role of the metal atom's position within the supercell.

- Customization Potential:

  Our calculations underscore the ability to customize both the band gap and magnetic behavior of GNMs by adjusting the type of doping and the position of the metal atom. This capability is valuable for the design of advanced semiconductor devices utilizing graphene materials.

- Conclusion:

  This study demonstrates that through careful selection of dopant metals and their positions within GNMs, it is possible to engineer materials with desirable electronic and magnetic properties for specific technological applications. The findings offer a pathway for the development of graphene-based materials with customized functionalities for use in spintronics and other electronic devices.