p-n codoping induced improvement of adsorption, magnetism, and electronic structure in 3d transition metal adatoms on graphene

SHIFEI QI, Shanxi Normal Univ. and Univ. of Science & Technology of China, ZHENYU ZHANG, Univ. of Science & Technology of China and Harvard Univ., XIAOHONG XU, Shanxi Normal Univ. — Generating ferromagnetism and preserving its unique properties in graphene are crucial to the development of graphene-based spintronics. Using first-principles calculations, we investigate the effects of p-n codoping method on absorption, magnetic properties, and of electronic structures 3d transition metal adatoms (TMs, i.e., Fe, Co, and Ni) on graphene. It is found that p-n codoping can strengthen the adsorption of TMs on graphene, and enhance the magnetic moments of Fe and Co adatoms on graphene. It can also cause Ni to transition from non-magnetic to magnetic states. Furthermore, magnetic coupling between two p-n pairs is also explored. Electronic structure analysis indicates that p-type dopant turns graphene into an electron-deficient system, and compensates for the shift in Fermi level caused by adsorption of TMs. Therefore, p-n codoping can bring about increases in the magnetic moment and adsorption of TM-adsorbed graphene systems while preserving the unique properties of graphene.

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