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**p-n codoping induced improvement of adsorption, magnetism, and electronic structure in 3d transition metal adatoms on graphene**[1] 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 nonmagnetic 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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