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A first-principles study on nonmetal and nonmagnetic metal atoms doped arsenene

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Recently, a new elemental 2D material has been identified based on theoretical calculations, namely grey arsenic, which is the structural counterpart of blue phosphorus. It can transform into an indirect band-gap semiconductor as thin as a monolayer (arsenene), which is different from planar graphene, silylene and puckered phosphorene. Interestingly, it can transform from indirect gap to direct gap semiconductor under biaxial strain and gets lots of attention. It has been verified that magnetism induced by the *sp* states of nonmetal elements has much stronger long-range exchange coupling interactions without clustering of magnetic ions. Therefore, we investigate the electronic and magnetic properties of X-doped arsenenes ($X =$ B, C, F, N, O, Al, Ga, Li, Mg, and Na), as shown in Fig. 1a, using first-principles method. Magnetic states are observed in the case of C. According to the binding energy, the C-doped arsenene is the most stable system, as shown in Fig. 1b. Then, we investigate the interaction between two C dopants and both nonmagnetic (NM) and antiferromagnetic (AFM) states were found. The projected density of states shows that the AFM order could be explained by the p–p coupling between C and its neighboring As atoms, as shown in Fig. 1c. Our study suggests that nonmetal dopant might be a possible approach to tune electronic and magnetic properties of arsenene [1–25].

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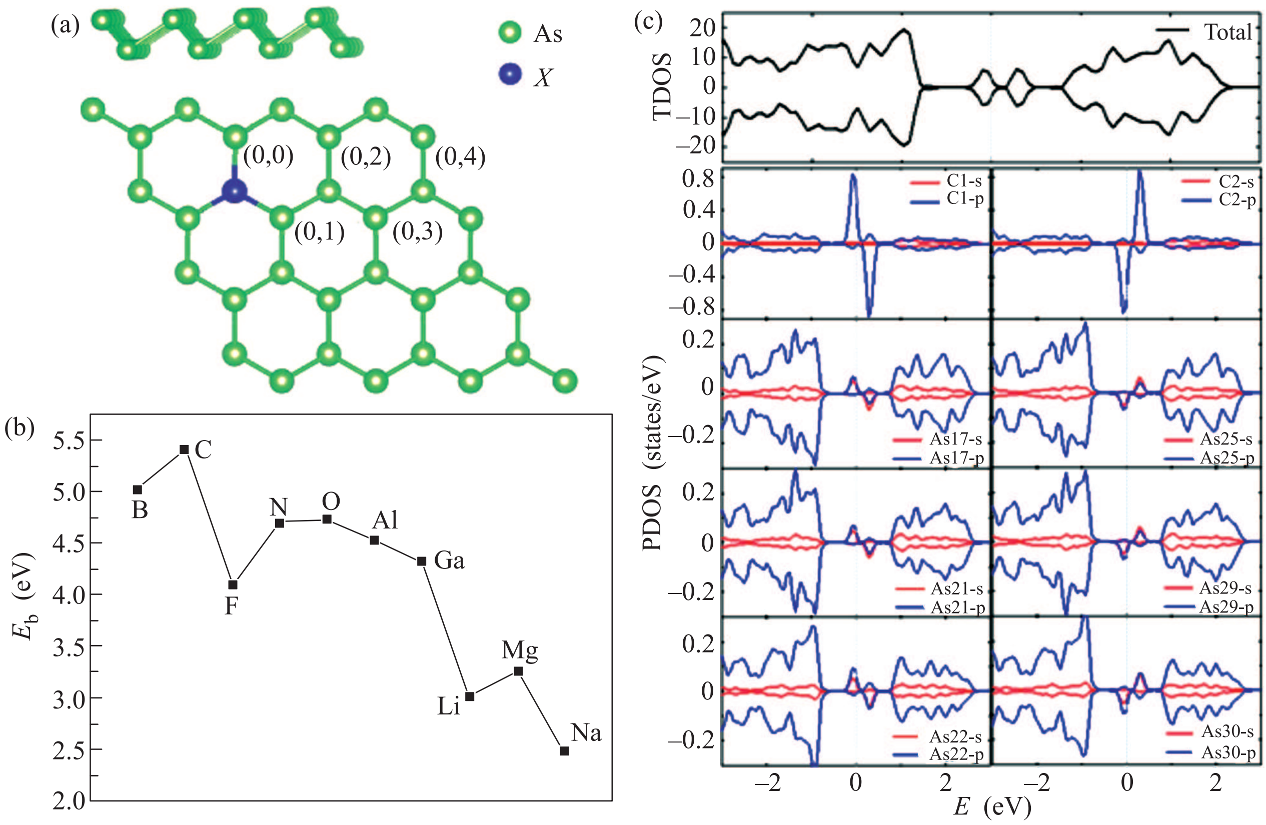

Fig. 1. (Color online) (a) – Top view of X-doped $4 \times 4 \times 1$ arsenene ($X =$ B, C, F, N, O, Al, Ga, Li, Mg, and Na). (b) – Binding energies of different nonmetals and nonmagnetic metals doped in the $4 \times 4 \times 1$ AsX, (c) – PDOS of two-C-doped system [case (0,4)]. The ground state is AFM

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