Pis'ma v ZhETF, vol. 104, iss. 8, pp. 575 – 575

A First-principles Study of Magnetic Properties in TM Atoms Adsorption on Arsenene

M. Luo[+1)], *Y. H. Shen*[*], *T. L. Yin*[*×]

[+]*Department of Electronic Engineering, Shang Hai Jian Qiao University, 201306 Shanghai, China*
[*]*Key Laboratory of Polar Materials and Devices, East China Normal University, 200241 Shanghai, China*
[×]*School of Electronics and Information, Nantong University, 226019 Nantong, China*

Submitted 5 September 2016

DOI: 10.7868/S0370274X16200078

Novel functional two-dimensional (2D) materials with unique and unpredictable features have become a hot for recent years. Arsenene as a new 2D semiconductor shows a wide band gap and gets lots of attention. A large number of researchers have given special attention to the properties of transition-metal (TM) doped 2D materials and TM atoms adsorption on 2D nanosheet also has been studied. In order to find its potential applications, we study TM (Co, Cu, Mn, Fe, and Ni) atoms adsorption on arsenene by using first-principles calculations. The first-principles method is based on density functional theory (DFT), which is implemented in the VASP package. In this paper, we investigate the magnetic properties of TM atoms adsorption on arsenene. As shown in Fig. 1a, b, there are three possible adsorption sites on the arsenene, which are labeled as TM1, TM2, and TM3, respectively. From our calculations, magnetism is observed in the cases of Co, Mn, and Fe. According to the adsorption energy, it is found that the stable adsorption site is TM3 for these three systems. Moreover, we also investigate the interaction in two TM (Co, Mn, and Fe) atoms adsorbed arsenene and several possible configurations of TM dopants are shown in Fig. 1c.

With increasing TM–TM distance, different magnetic behavior appears, as shown in Fig. 1d. Both nonmagnetic and ferromagnetic states are found in two-Co-adsorbed system, which could be explained by the $p-d$ hybridization mechanism. But in the cases of Mn and Fe, the superexchange dominates other exchange and an AFM interaction with null spin polarization is observed. Such multiple magnetic properties have never been reported in 2D materials before. Our work suggests some potential applications of TM-adsorbed arsenene in electronics and spintronics.

Full text of the paper is published in JETP Letters journal.

DOI: 10.1134/S0021364016200029

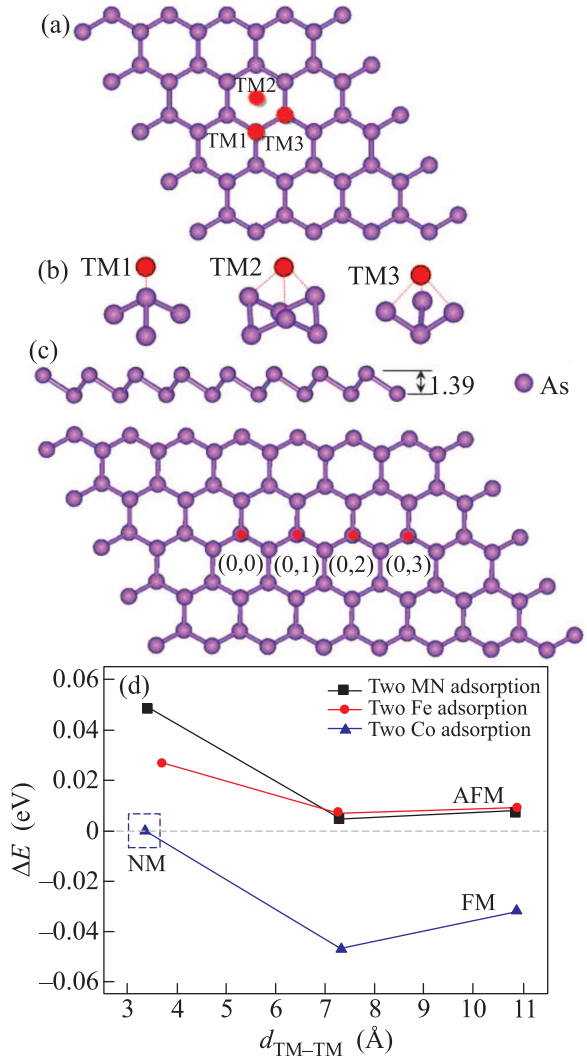

Fig. 1. (Color online) (a) – Top view of three different adsorption sites in the $5 \times 5 \times 1$ supercell. (b) – Side view of the adsorption sites, marking as TM1, TM2 and TM3, respectively. (c) – The configurations of two TM (Mn, Fe, and Co) atoms adsorption on the $8 \times 5 \times 1$ arsenene. (d) – The total energy difference (ΔE) as a function of TM–TM distance. Inside dashed square is nonmagnetic (NM) state

[1)]e-mail: mluo@gench.edu.cn