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The electronic structure calculations of Fe doped monolayer MoS_2 using density functional theory

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Recently, the single-layer two-dimensional (2D) of MoS_2 is an important transition metal dichalcogenides (TMDs) compound which has been investigated [1,2]. Similar to the graphene, the monolayer of MoS_2 is used in a wide range of application including field-effect transistors, photodetectors, solar cells, chemical sensors and supercapacitors electrodes [3,4]. Furthermore, due to the relatively high direct band gap of 1.8 eV in the monolayer MoS_2, it has great advantage respect to the graphene that can be used as a host material for transition metal implantation.

In this work, the magnetic and electronic properties of monolayer MoS_2 doped with Fe atoms have been investigated by first-principle calculations in the framework of density functional theory (DFT) based on the full-potential linear augmented plane wave (FPLAPW) method as implemented in the wien2k code [5]. The various configurations of Fe doped MoS_2 (*I.* Substitutional Fe doped Mo site, *II.* Substitutional Fe doped Mo site with vacancies of S atom, *III.* Interstitial Fe on the surface of monolayer MoS_2) have been stimulated. The charge state of Fe and the density of states of each configurations are discussed.

The results of this work provide information about the change of the electronic structure in the monolayer MoS_2 with different implanted Fe site.

References:
[1] Lin, Xianqing, and Jun Ni. "Charge and magnetic states of Mn-, Fe-, and Co-doped monolayer MoS_2." Journal of Applied Physics 116.4 (2014): 044311.
[2] Cui, Zhen, et al. "Alkali-metal-embedded in monolayer MoS_2: optical properties and work functions." Optical and Quantum Electronics 50.9 (2018): 348.
[3] Zhang, Yijin, et al. "Ambipolar MoS_2 thin flake transistors." Nano letters 12.3 (2012): 1136-1140.
[4] Schmidt, Hennrik, et al. "Transport properties of monolayer MoS_2 grown by chemical vapor deposition." Nano letters 14.4 (2014): 1909-1913.
[5] Blaha, Peter, et al. "wien2k." An augmented plane wave+ local orbitals program for calculating crystal properties (2001).

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