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Electronic and magnetic properties of Selected TM doped MoS2 monolayer: A DFT calculation

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The exfoliation of free-standing graphene in 2004 had led to several other monolayered materials synthesis and characterization, of which Molybdenum disulfide (MoS2) is one of them. MoS2 has superior physical and electronic properties comparable to that of graphene and candidate material for next generation device materials application since its semiconducting while graphene is semimetal. In addition, MoS2 has a good potential application in nanoelectronics, optoelectronics, and flexible devices. It has the capability of controlling spin and valley degrees of freedom making it a promising material for spintronic and valleytronic devices. Monolayer MoS2 by its nature is nonmagnetic, and it has been reported that using electron beam mediated substitutional doping, transition metals (TM) can alter the electronic and magnetic properties of MoS2 monolayer. Vacancy defects have also been found to induce magnetic properties under Molybdenum rich conditions extending the magnetic applications of MoS2 from the experimental point of view. TM doped MoS2 and vacancy creations are promising ways to induce magnetic effect in MoS2 and to achieve that, we examine the combined effect of both localized (TM= V, Ni, Fe Cu and Mn)-vacancies of MoS2 using quantum mechanical approach in the framework of density functional theory with generalized gradient approximation. The results demonstrate that, it is energetically stable to incorporate Ni and Cu in MoS2 structure under Mo-rich conditions than others. There are observed induced magnetic effects originating from the dopants and the nearest-neighbour Mo with magnetic moments between 0.82 and 3.00 μB. Some of the dopants showed 100% spin polarization which is useful for engineering spin filter devices on magnetic MoS2 nanostructures.

The results reported here are certainly important and interesting, and will contribute to the present knowledge in the field of spintronics.

Keys works: transition metal, monolayer, spin and magnetic properties

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Abstract Category

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