The Effects of Different Dopant Separation on Electronic States and Magnetism of MoS$_2$

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Abstract

Doping is another effective method to modulate the electronic and magnetic properties of materials. The atoms of monolayer MoS$_2$ are highly exposed, which is very favorable for doping. The effects of vanadium (V) dopant on the electronic and magnetic properties of monolayer MoS$_2$ are investigated by first principles calculation. The substitutionally doped V produces antiferromagnetic (AFM) or ferromagnetic (FM) states depending on the separation between V dopants. When the separation between V dopants is smaller than 6.38 Å and the maximum dopant concentration is 25%, the superexchange interaction between V atoms is stronger than the double exchange interaction between the localized V $3d$ orbitals and Mo $4d$ orbitals, resulting in the AFM state in monolayer MoS$_2$. However, the double exchange interaction between the V and Mo atoms becomes stronger than the superexchange interaction between V atoms if the separation between V dopants is larger than 9.57 Å when the maximum dopant concentration is 11.11%. Consequently, the FM state is observed from the monolayer MoS$_2$ and 100% spin polarization takes place if the separation between V atoms is further increased to 12.76 Å at a dopant concentration of 6.25%. The transition is mainly due to the competition between the double exchange between V and Mo and the superexchange between V atoms. The results suggest potential applications of monolayer MoS$_2$ as diluted magnetic semiconductors (DMS) in spintronics.