Magneto-crystalline Anisotropy of mono-layer VSi_2P_4

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First-principles calculations based on density functional theory (DFT) for spin polarized and non-collinear magnetism with DFT+U and DFT+U+SOC are carried out to study the electronic structure, magnetism, and magneto-crystalline anisotropy (MCA) of mono-layer VSi_2P_4. The magneto-crystalline anisotropy energy is calculated for ML VSi_2P_4 at different applied bi-axial strains. At equilibrium, VSi_2P_4 is a ferromagnetic semiconductor. The calculated band gap for majority-spin and minority-spin is 0.24 eV and 0.26 eV, respectively. The electronic properties changes with applied strain. Within the compressive strain range of 0% to -2%, VSi_2P_4 shows ferromagnetic metallic behavior. Subsequently, as the tensile strain increases from 0% to 4%, it change into a ferromagnetic semiconductor. Finally, with tensile strain increase from 4% to 6%, it becomes half metal ferromagnet. The equilibrium MCA is 0.065 meV/magnetic atom. Positive MCA energy indicates the in-plane magnetic anisotropy. With applied strain, the MCA energy increase from 0.02 meV/ magnetic atom to 0.098 meV/ magnetic atom. We show that VSi2P4 is a magnetic semiconductor with in-plane magnetic anisotropy.

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