Effect of strain on the electronic and magnetic properties of bilayer T-phase VS_2: a first-principles study

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We will discuss the electronic and magnetic properties of the bi-layer of Vanadium disulfide (VS_2) in an octahedral (1T) phase. Using the Density Functional Theory (DFT), we have found that the ground state of VS_2 bilayer structure is antiferromagnetic (AFM) without taking Hubbard correction $U = 0$, however it becomes ferromagnetic with $U = 2$ eV. This shows a high sensitivity of this structure to the on-site Coulomb interaction. Moreover, subsequent spin-resolved band structures in the presence of U and spin-orbit coupling (SOC) show a metallic behavior for the pure structure.

We will also discuss the calculated exchange parameters (J_{ij}) that are crucial for understanding the magnetic behavior of the T-phase VS_2. In addition, we used the calculated exchange parameters to calculate the Curie temperature (within the mean-field approximation as well as random phase approximation) and magnon band structures.

As the calculated magnon band structure is also affected by the spin-orbit coupling (SOC), we have also calculated the Dzyaloshinski-Moriya parameters and the Magnetic Anisotropy Energy (MAE) of the bilayer structure. Our results show that the MAE is equal to -0.0610 meV, indicating an in-plane easy axis of magnetization.

Finally, we will discuss also the impact of bi-axial strain (ranging from -10% to $+10\%$) on the magnetic and electronic properties of the T-phase VS_2. Our results show that the magnetic and electronic properties of T-phase VS_2 are highly sensitive to the strain, with significant changes observed in the band gap, magnetic moment, J_{ij} parameters, Curie temperature, and magnon band structure. The ability to tune the magnetic and electronic properties of the T-phase VS_2 by strain engineering makes it a promising candidate for various applications, including magnetic memory devices, spintronics, and magnetic sensors [1-3].

References:

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