Supplemental Material for

Ferromagnetic vanadium disulfide VS_2 monolayer with high Curie temperature and high spin polarization

Hao-Jia Wu [1], Yu-Lu Wan[1], Zhao-Yi Zeng [2], Cui-E Hu [2,*], Xiang-Rong Chen [1,*], Hua-Yun Geng [3]

[1] College of Physics, Sichuan University, Chengdu 610064, China;

[2] College of Physics and Electronic Engineering, Chongqing Normal University, Chongqing 400047, China;

[3] National Key Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, CAEP, Mianyang 621900, China

Abstract: The structural, electronic, and magnetic properties of vanadium disulfide VS_2 monolayer were investigated by first-principles calculation and Monte Carlo (MC) simulations. The results of molecular dynamics simulations and phonon dispersion showed that the VS_2 monolayer has good dynamic and thermodynamic stabilities. Based on the results of band structure, we also explore the effect of carrier concentrations on the spin gap, spin polarization and the direction of the easy magnetic axis. Our results demonstrated that the doping appropriate amount of holes can cause the reversal of easy magnetic axis and maintain nearly 100% spin polarization, which greatly improves the application possibility of the VS_2 monolayer as a spintronic device. The contribution of different orbits to spin-orbit coupling (SOC) effect is given

* Corresponding authors. E-mail: cuiehu@cqnu.edu.cn; xrchen@scu.edu.cn

in magnetocrystalline anisotropy energy, which provides a theoretical basis for explaining the origin of magnetic crystal anisotropy. Based on the MC simulations, we also showed the influences of different parameters (carrier concentrations, magnetic field and crystal field) on the magnetothermal properties of the VS_2 monolayer. It is found that the increase of hole doping concentrations can promote the increase of the Curie temperature; while the increase of electron doping concentrations will greatly weaken the Curie temperature. Furthermore, according to the influences of different parameters on Curie temperature and spin polarization, we concluded that properly enhanced magnetic field and hole concentrations will not only make the system maintain high spin polarization, but also make the system show ferromagnetic properties higher than room temperature.

Keywords: Electronic structure; Magnetic properties; Spin polarization; Curie temperature; Magnetocrystalline anisotropy energy

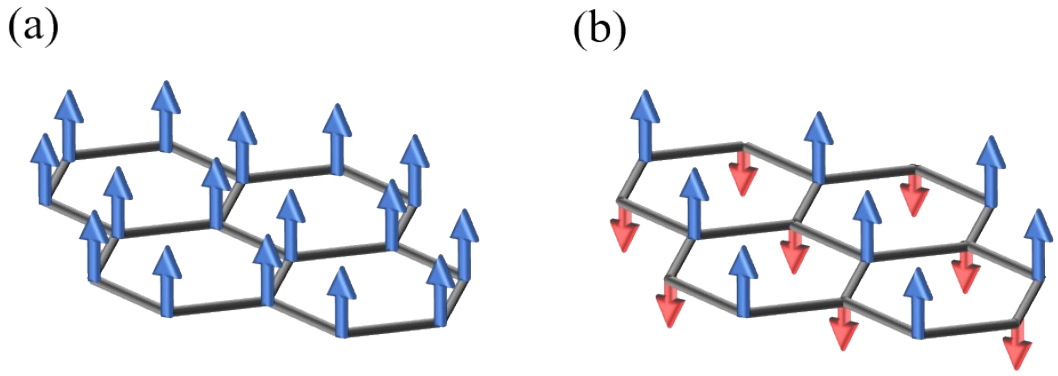

Fig. S1 (Color online) (a) The ferromagnetic configuration of VS_2, where the total energy can be written as: $E_1 = E_0 - \frac{1}{2}\cdot\frac{1}{2}\cdot\frac{1}{2}\cdot 3\cdot 16\cdot J = E_0 - 6J.$ (b) Antiferromagnetic configuration of VS_2, where the total energy can be written as: $E_2 = E_0 + \frac{1}{2}\cdot\frac{1}{2}\cdot\frac{1}{2}\cdot 3\cdot 16\cdot J = E_0 + 6J$. Here, E_0 is the total energy excluding the magnetic coupling and 16 represents the number of magnetic atom (V) in the unit cell, and $J = \frac{E_2 - E_1}{12}$.

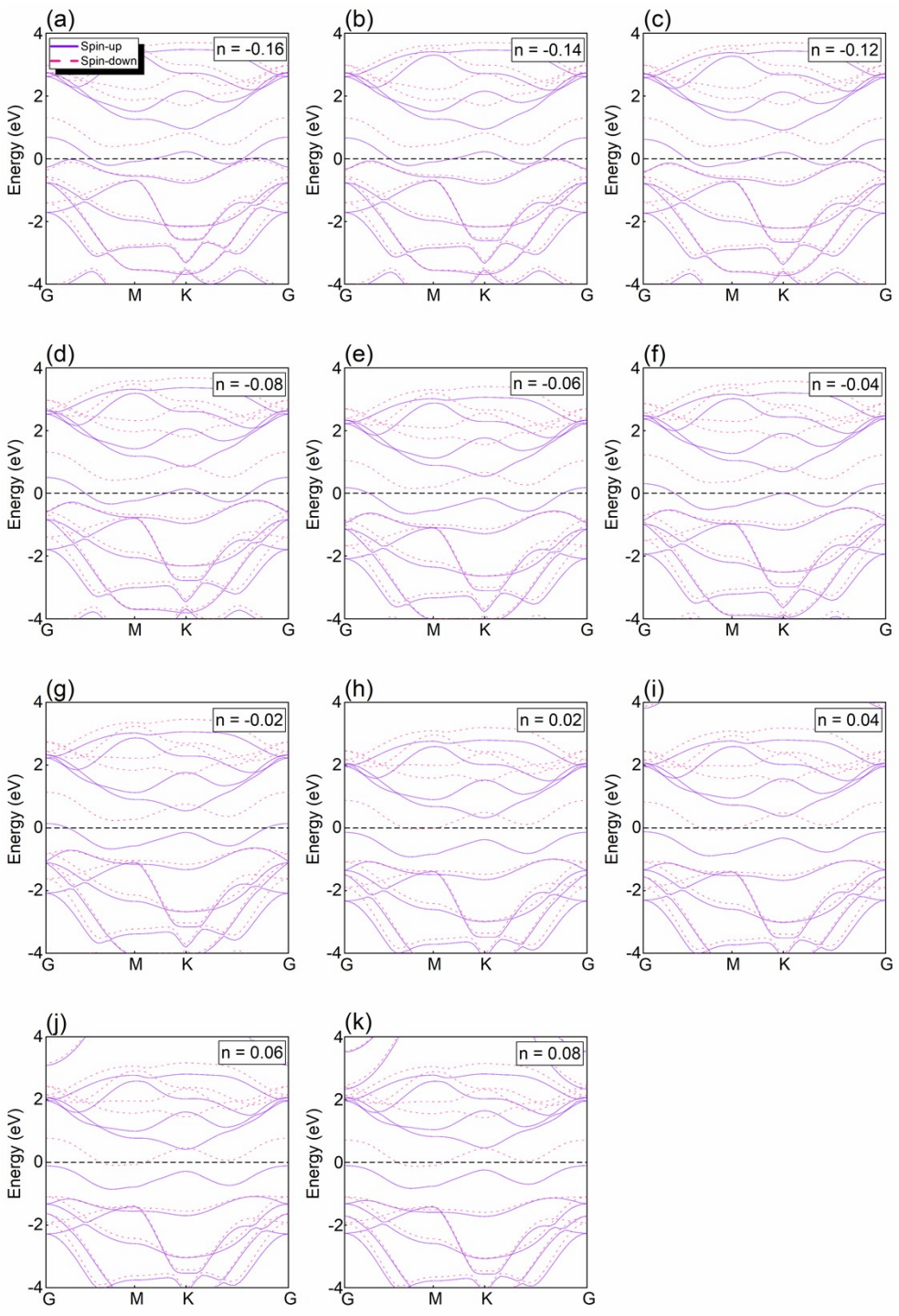

Fig. S2 (Color online) (a)-(g) Band structure at different hole concentrations; (h)-(k) Band structure at different electron concentrations. The purple lines represent spin-up bands and the red lines represent spin-down bands.