Magnetic properties of TRS broken ferrovalley semiconductors

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ABSTRACT

The intrinsic ferromagnetism in 2D materials and the magnetic anisotropy energy (MAE) are importants yardstick for nanoscale applications. We employed first-principles scheme to investigate the electronic band structures, the strain dependence of MAE in pristine VSi_2Z_4 (Z=P, As) and its Janus phase $VSiGeP_2As_2$ and the evolution of the topology as a function of the Coulomb interaction. It is observed that $MoSi_2P_4$ monolayer show equal bandgaps at K/K′ points of brillouine zone due to the the preserved time-reversal symmetery (TRS). On the other hand, all the vanadate based 2D structures exhibit unequal bandgaps at K/K′ with ferromagnetic ground state ordering owing to broken TRS, which is known as ferrovalley semiconductors. A large value of coupling J is obtained, and this, together with the magnetocrystalline anisotropy can produce a large critical temperature. We found an out-of-plane (in-plane) magnetization for VSi_2P_4 (VSi_2As_4), while in-plane magnetization in $VSiGeP_2As_2$. Furthermore, we observed a correlation-driven topological transition in the Janus $VSiGeP_2As_2$. These ferrovalley semiconductors possess inherent spontaneous valley polarization induced by intrinsic ferromagnetism and, thus offer the possibility to address the challenges of valleytronic materials.