Tuning spin-momentum locking in magnetic transition metal di-chalcogenide Janus monolayers

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Abstract
Among the vast zoology of novel two-dimensional materials, transition metal dichalcogenide monolayers stand out as a versatile platform for the advancement of disruptive flat microelectronics and spintronics [1-5]. Indeed, in contrast to graphene some transition metal dichalcogenides possess a large band gap that promotes optoelectronic operation and the realization of light-driven spin-valley coupling [6]. Alternatively, transition metal dichalcogenide monolayers with 3*d* elements tend to be metallic and exhibit magnetism. As such, they constitute a promising candidate for ultrathin magnetic memories operated by spin-orbit torque, a novel approach enabling the electrical control of magnetization exploiting spin-orbit coupling in a material lacking inversion symmetry [7].

In the present work, we have investigated the magnetic properties, magnetic anisotropy and electronic structure of a series of Vanadium dichalcogenide monolayers using first principle calculations. We find that the magnetism and magnetic anisotropy increase upon changing the chalcogen from S to Te, and scale with the orbital momentum. We explain this behavior by the reduced charge transfer between the transition metal and the chalcogen elements. Most remarkably, we have extended this study to so-called Janus monolayers, i.e., systems where Vanadium sits in-between dissimilar chalcogens. This approach breaks the inversion symmetry of the monolayer, enabling the emergence of Rashba-like spin-orbit coupling, which can promote spin-orbit torques. By projecting the band structure on the spin states using Wannier interpolation method, we observe large spin-momentum locking, which we explain in terms of asymmetric orbital overlap. This discovery opens fascinating perspectives for ultrathin magnetic memories.

Figures

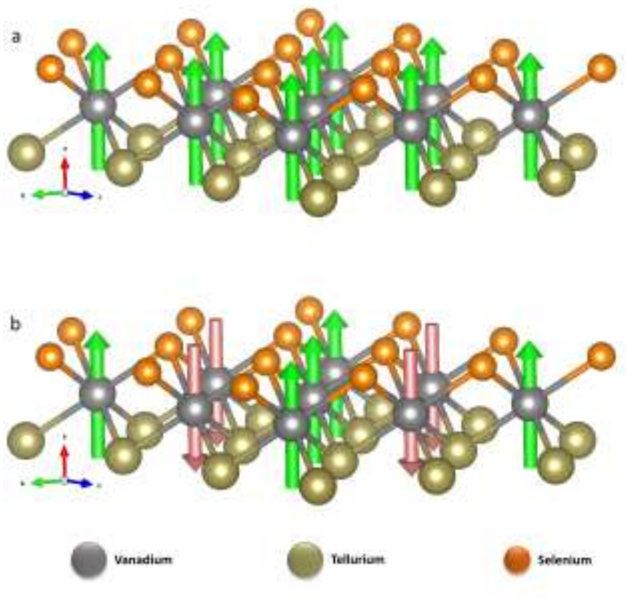

Figure 1: 2x2x1 VSeTe monolayer with corresponding magnetic moments (a) Ferromagnetic (b) Antiferromagnetic

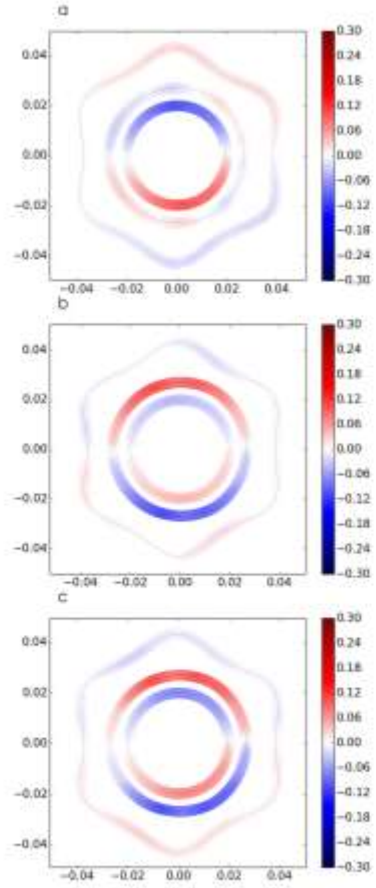

Figure 2: Spin textures of VSeTe monolayer (a) S_x of V (b) S_x of Se (c) S_x of Te

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