Valley polarization in magnetically doped single layer transition metal dichalcogenides

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Abstract

The fields of electronics and spintronics require an active control and manipulation of the charge and spin degrees of freedom [1]. Valleytronics, on the other hand, is very new field that relies on the property that the conduction/valence bands have two or more minima/maxima at equal energy but different momenta. For valleytronics devices it is necessary to induce valley polarization, i.e., control the number of electrons in each valley, typically by strain [2] or a magnetic field [3, 4]. In general, two-dimensional materials have raised a lot of interest both for fundamental and applied reasons. Examples are semiconductor quantum wells [5], noble metal surfaces [6], graphene [7], and topological insulators [8]. Semiconducting single layer transition metal dichalcogenides MX_2 with M = Mo, W and X = S, Se, Te and D_{3h} point group have caught attention, because they display distinctively different physical properties as compared to their bulk compounds with D_{6h} point group. There exists a crossover from an indirect band gap in multilayers to a direct band gap in the single layer limit [9-12], see Fig. 1(a). In the latter the conduction and valence band edges are located at the K points of the two-dimensional hexagonal Brillouin zone, see Fig. 1(c). These two inequivalent valleys constitute a binary index for low energy carriers, which gives rise to a valley Hall effect and valley dependent optical selection rules for interband transitions at the K points [13-15]. It has been demonstrated that optical pumping with circularly polarized light can achieve a dynamic valley polarization in single layer MoS_2 [16-18]. From application point of view, the equilibrium valley polarization in single layer MX_2 is more important, which has not been investigated till now experimentally or theoretically.

The interplay between spin orbit coupling and ferromagnetism in two-dimensional materials gives rise to a variety of unconventional phenomena, such as the quantum anomalous Hall effect [19-22]. In addition, it recently has been put forward that dichalcogenides doped with magnetic transition metal atoms form a promising platform for two-dimensional dilute magnetic semiconductors [23-25]. However, these studies did not take into account the spin orbit coupling, which interconnects the spin and valley physics, making it desirable to investigate the effects of the exchange field induced by magnetic doping.

We propose in this work a method to control the valley polarization by magnetic doping, see Fig. 1(b,d, and e). Various possible Mn doping sites in single layer MoS_2 are studied to investigate the influence of the exchange field on the electronic structure by first-principles calculations. We will argue that the strength of the spin orbit coupling together with the exchange energy determine the valley polarization, which can be inverted by modifying the spin polarization.

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Figures

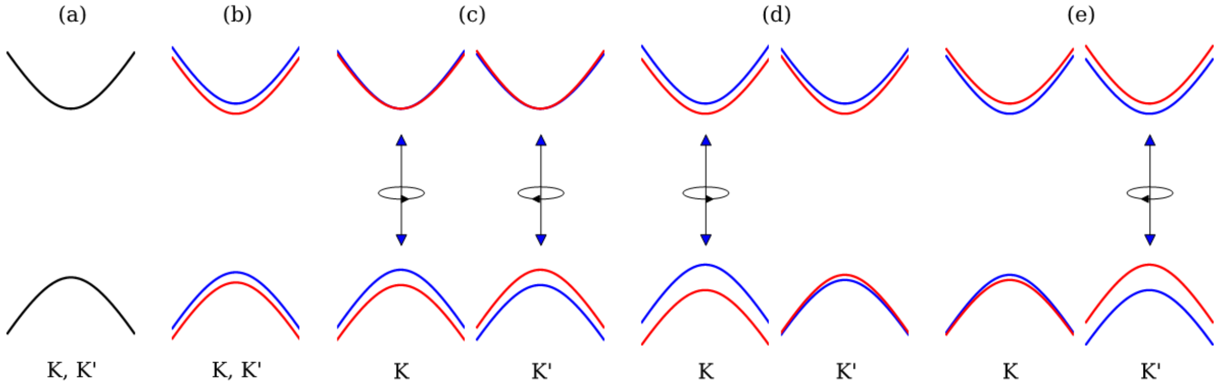

Figure 1. Schematic view of the band structure of single layer MoS_2 near the K and K' points: (a) pristine without spin orbit coupling, (b) with exchange field and without spin orbit coupling, (c) pristine with spin orbit coupling, and (d) with exchange field and with spin orbit coupling. (e) Same as (d) but with inverted spin polarization.