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Valley polarized magnetic state in hole-doped monolayers of transition metal dichalcogenides

Spontaneous valley polarization was predicted and experimentally confirmed over thirty years ago for Si inversion layers [1,2]. The isolation of real 2D materials with hexagonal lattice like graphene has put valley physics in the spotlight again; yet, the manipulation of the two valleys of graphene is not easy to achieve [3]. Such manipulation has been demonstrated for the class of 2D materials known as semiconducting transition metal dichalcogenides (TMDs) [4]. In this work, we predict that hole doped TMDs, in particular those with large spin-splitting of the valence band like WS_2, display a valley polarized ferromagnetic (VPF) phase. A typical phase diagram is shown in Figs. 1(a) and (b), in the plane of intra-orbital U Coulomb interaction and hole density n_{hole}, and in the plane of U and inter-orbital U' interaction, respectively. The valence band in the normal and VPF phases are respectively plotted in Figs. 1(c) and (e), showing how the sizable spin-splitting couples the valley and spin degrees of freedom. The VPF phase lifts the degeneracy of the inequivalent valleys, polarizing the material in the two degrees of freedom. This degeneracy lifting allows for anomalous Hall (AH) responses [5], in virtue of the Berry curvature of these bands [6]. We predict an AH response that is proportional to the Berry curvature at the K points and to the total magnetization density of the system. This response is simultaneously valley- and spin-polarized, thus providing a measurable signature of the VPF phase. This work is currently in pre-print [7].

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Figures

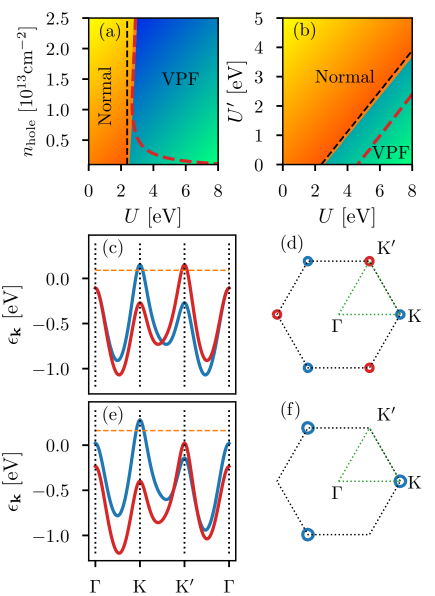

Figure 1: (a) Mean field phase diagram in the n_{hole}–U plane, indicating the normal and VPF phases, at a temperature of T=1K and U'=0 for the TMD WS_2. The dashed red line indicates the transition at T=100K. The vertical dashed line represents the estimated critical U of 2.38 eV in the limit of low T and n_{hole} obtained using a low energy model. (b) Phase diagram in the U–U' plane at a hole density of n_{hole}=0.2×10^{13} cm^{-2} and T=1K. The dashed red line shows the transition line at the temperature of T=100K. The dashed black line indicates the critical line U=U_c+1.4U', estimated using the low energy model. Panels (c) and (e) show the band structure for the spin up (in red) and spin down (in blue) valence bands in the normal and VPF phases, respectively. The horizontal dashed line indicates the Fermi level for a constant particle number of n_{hole}=0.2×10^{13} cm^{-2}. The Fermi surfaces for the normal and VPF phases are represented in panels (d) and (f), respectively.