Tunable valley splitting in 2D MPX_3 crystals.

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Valleytronics has attracted a great interest in 2D materials, due to number of intriguing properties such as spin-valley locking and valley Hall effect [1]. Tailoring valley degrees of freedom offers unique playground to realize pecular phenomena and novel applications, Here, we have demonstrated that the monolayer of transition metal trichalcogenides $MnPX_3$ (X=S, Se), which are layered antiferomagnts [2,3], could be viewed as promising valley electronics materials. In particular, we have shown that the valley splitting at the K+/K- can be effectively control by the direction of the magnetic moments. In particular, the sizable valley splitting occurs for the out-of plane direction of the magnetic moments in monolayer of MnPSe3, resulting in valley dependent gaps, as it is presented in Fig. 1. On the other hand, the valley dependent gaps rely on the type of the chalcogen atoms. Moreover, the K+/K- valleys are spin degenerated, which might hinder their spintronic applications. Hence, we have also propose a novel way how the valley polarization can be achieved. We have suggested that particular deformation of the hexagonal lattice of $MnPX_3$ could lead to the spin resolved valley splitting. Our results give insight into the valley splitting realization in 2D antiferromagnets.

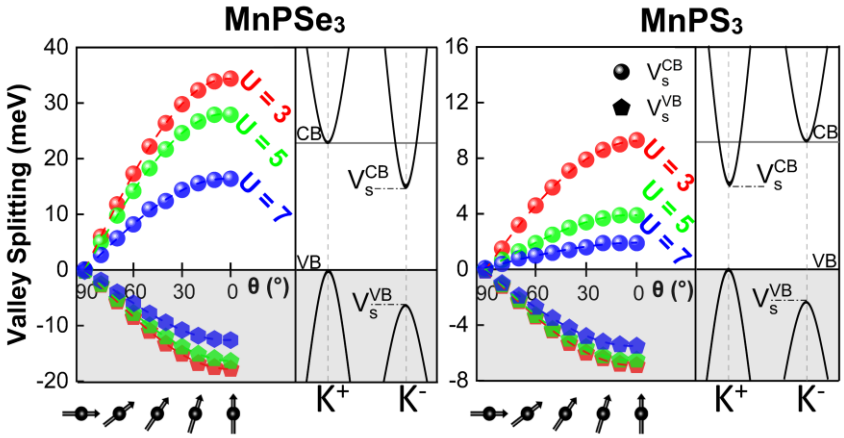

Fig. 1. Tunable Valley splitting upon the change of the direction of Mn spins from the in-plane to out-of plane direction.

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[1] J. R. Schaibley, 2016. "Valleytronics in 2D materials". United States.
[2] B. L. Chittari et al. Phys. Rev. B 94, 184428 (2016).
[3] M. Birowska, et al. Phys. Rev. B 103, L121108 (2021)