Magnetic signatures in structural, electronic and optical properties of 2D MPX_3 crystals

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Since recent years the magnetism in two-dimensional (2D) materials has emerged as one of rapidly growing research areas, with many exciting properties and potential applications in low-power spintronics, and optical communication [1]. The current study focuses on the transition metal phosphorous trichalcogenides semiconductors (MPX_3, M=Mn, Ni, Fe, X=S, Se), which are layered antiferromagnetic semiconductors. These materials are stable in air and exhibit facinating properties, such as recenlty predicted giant excitionic binding energies sensitive to the polarization of light [2].

In this report, we adress a following scientific questions: what mechanism sustains the long-range AFM ordering, and whether the type of magnetic arrangement can be manipulated? Here, we report a comprehensive theoretical *ab initio* results of the structural, electronic and optical properties of the series of MPX_3 monolayers (M=Mn, Ni, Fe, and X=S,Se). We also present the results for alloy systems with magnetic [3] and nonmagnetic substitution [4]. In particular, for the AFM-Neel magnetic ordering, the inclusion of the spin-orbit interaction (SOI) causes an in-equivalency of the pair of valleys (K+,K-), resulting in sizeable valley splitting, which can be tuned by the rotation angle of the spins. In the case of $MnPS_3$, $MnPSe_3$ and $FePS_3$ monolayers, we have demonstrated that the band edge direct transitions are optically active and sensitive to the polarization of light. In addition, our results reveal an effective tuning of magnetic interactions and anisotropies in both $MnPS_3$ and $NiPS_3$ upon nonmagnetic substitution [4]. Finally, we highlight the importance of the structural anisotropy in monolayer of $FesPS_3$, resulting in local inversion symmetry breaking, leading to lifted spin degeneracy of K+/K- valleys, and two optically active transitions visible in experiments [5]. Such efficient engineering of the magnetism in MPX_3 materials provides a suitable platform to understand the magnetism in thin samples

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