Various anisotropies in atomically thin AFM MPX_3 crystals

M. Rybak[3], T. Woźniak[1], P. Scharoch[3] and M. Birowska[1]

[1] *University of Warsaw, Faculty of Physics, Pasteura 5, 00-092 Warsaw, Poland*
[3] *Department of Semiconductor Materials Engineering Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland.*

Anisotropy is the characteristic feature of a material referring to different physical properties along different directions. Generally, it is an intrinsic property related to atomic structure. The layered materials are naturally anisotropic, as they missing the third dimension. The two-dimensional (2D) materials frequently occurring as an isotropic materials such as widely examined graphene or TMDs. However, the in-plane anisotropy can also occur, or can be induced by various factors such as strain, defects, stacking order, external magnetic or electric fields.

In this work, by used of the density functional theory (DFT), we reveal an occurrence of in-plane anisotropic features in the magnetic, electronic, transport, and optical properties in monolayers of transition metal phosphorus trisulfides (MPX_3, M=Mn, Ni, Fe, X=S, Se) [1-4]. These materials are 2D antiferromagnetic (AFM) crystals. We have shown, that $FePS_3$, exhibit structural anisotropy stemming from breaking of the hexagonal symmetry of magnetic ions, resulting particularly in magnetoelectric anisotropies [1]. Additionally, we have determined the optically active band edge transitions (Mn,Fe)PX_3, predicting that they are sensitive to in-plane magnetic order [2]. We have revealed linear polarization as an important fingerprints for sensing the type of magnetic AFM arrangements. Additionally, we identify the spin-orientation-dependent features such as the valley splitting, the effective mass of holes, and the exciton binding energy. In particular, we demonstrate that for $MnPX_3$ (X=S, Se) a pair of non equivalent K+ and K- points exists yielding the valley splittings that strongly depend on the direction of AFM aligned spins. These features can be referred as sensitive parameters that provide insight into spin flop transitions.

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