Monolayer and bilayer $PtSe_2$: spin orbit-coupling, spin relaxation and twisting.

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Monolayer $PtSe_2$ is a semiconducting transition metal dichalcogenide characterized by an indirect band gap, space inversion symmetry, and high carrier mobility. Strong intrinsic spin-orbit coupling and the possibility to induce extrinsic spin-orbit fields by gating make $PtSe_2$ attractive for fundamental spin transport studies as well as for potential spintronics applications. We perform a systematic theoretical study of the spin-orbit coupling and spin relaxation in this material. Specifically, we employ first principles methods to obtain the basic orbital and spin-orbital properties of $PtSe_2$, also in the presence of an external transverse electric field. We calculate the spin mixing parameters b^2 and the spin-orbit fields Ω for the Bloch states of electrons and holes. This information allows us to predict the spin lifetimes due to the Elliott-Yafet and D'yakonov-Perel mechanisms, which we estimate to be on the picosecond level. We compare $PtSe_2$ to other transition metal dichalcogenides, such as WS_2 or MoS_2. Effects of twisting in bilayer $PtSe_2$ on electronic and optical properties are also discussed.

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