Gate Tunable Nonlinear Rashba spin splitting in transition metal dichalcogenide monolayers

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Abstract:

Single-layer transition-metal dichalcogenides (TMD) such as MoS₂ and MoSe₂ have unique electronic band structures, ideal for hosting many exotic spin-orbit phenomena such as Rashba effect. It has been widely accepted that Rashba-type spin splitting (RSS) is linearly proportional to the external gate electric field in metallic heterostructure interface or to potential gradient in polar materials. Here an extraordinary nonlinear dependence of RSS is surprisingly found in semiconducting TMDs monolayers under gate field using first-principles calculations. In contrast to a small, constant RSS in polar materials, the electrostatic potential gradient in non-polar TMDs gradually increases with gate voltage, resulting nonlinear RSS with a Rashba coefficient an-order-of-magnitude larger than that for materials of similar elemental mass. Based on a **k-p** model via symmetry analysis, we identify that the third-order anisotropic contribution is responsible for the extra-large nonlinear Rashba splitting. The gate tunable spin splitting found in semiconducting pristine TMD monolayers promises for future spintronics applications in that spin polarized electrons can be generated by external gating in an experimentally accessible way.