Highlights

Innovative materials with strong interplay of spin orbital charge and topological degrees of freedom - 2018

Intrinsic and anisotropic Rashba spin splitting in Janus transition-metal dichalcogenide monolayers

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Transition-metal dichalcogenides (TMD) monolayers are important two-dimensional materials for the study of fundamental physics in the field of spintronics. Recently, a newly synthesized Janus TMD MoSSe was found to intrinsically possess both the in-plane inversion and the out-of-plane mirror-symmetry breaking. Here we performed first-principles calculations in order to systematically investigate the electronic band structures of a series of Janus monolayer TMD with chemical formula MXY (M = Mo,W and X,Y = S, Se, Te). We found that they possess robust electronic properties like their parent phases. We explored also the effect of perpendicular external electric field and in-plane biaxial strain on the Rashba spin splittings. The Zeeman-type spin splitting and valley polarization at K(K′) point are well preserved and we observed a Rashba-type spin splitting around the Γ point for all the MXY systems. We have also found that these spin splittings can be enhanced by an external electric field collinear with the local electric field due to the presence of polar bonds and by the compressive strain. The Rashba parameters change linearly with the external electric field, but nonlinearly with the biaxial strain. The compressive strain is found to enhance significantly the anisotropic Rashba spin splitting.

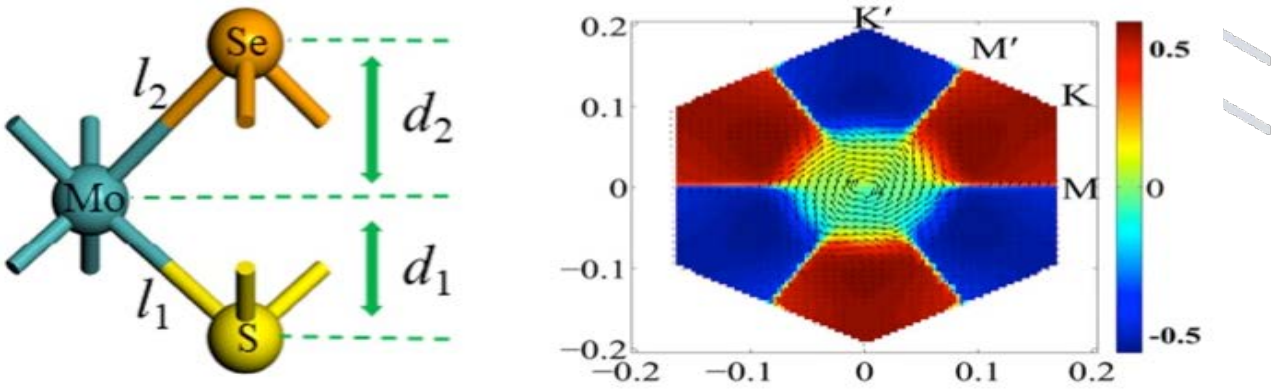

Fig.1: (Left side) Top and side views of the unit cell of MoSSe monolayer. (Right side) Spin texture of the valence band maximum (VBM) at the K point and the VBM around Γ point. The arrows corresponds to the in-plane spin vector orientation and the colors indicate the out-of-plane component of the spin.