First-principles insights into the spin-valley physics of strained transition metal dichalcogenides monolayers

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Transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of spin-valley physics under external stimuli. Here, we investigate the influence of strain on the spin and orbital angular momenta, effective g-factors, and Berry curvatures of several monolayer TMDCs (Mo and W based) using state-of-the-art first principles calculations of the spin and orbital angular momenta[1-4]. At the K-valleys, we find a surprising decrease of the conduction band spin expectation value for compressive strain, consequently increasing the dipole strength of the dark exciton by more than one order of magnitude. We also predict the behavior of direct excitons g-factors under strain: tensile (compressive) strain increases (decreases) the absolute value of g-factors. Strain variations of ~ 1% modify the bright (A and B) excitons g-factors by ~ 0.3 (0.2) for W (Mo) based compounds and the dark exciton g-factors by ~ 0.5 (0.3) for W (Mo) compounds. Our predictions could be directly visualized in magneto-optical experiments in strained samples at low temperature. Additionally, our calculations strongly suggest that strain effects are one of the possible causes of g-factor fluctuations observed experimentally. By comparing the different TMDC compounds, we reveal the role of spin-orbit coupling (SOC): the stronger the SOC, the more sensitive are the spin-valley features under applied strain. Consequently, monolayer WSe_2 is a formidable candidate to explore the role of strain on the spin-valley physics (summarized in Fig.1 for the K-valley). We complete our analysis by considering the side valleys, Γ and Q points, and by investigating the influence of strain in the Berry curvature. In the broader context of valley- and strain-tronics, our study provides fundamental microscopic insights into the role of strain in the spin-valley physics of TMDCs, which are relevant to interpret experimental data in monolayer TMDCs as well as to model TMDC-based van der Waals heterostructures.

References

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Figures

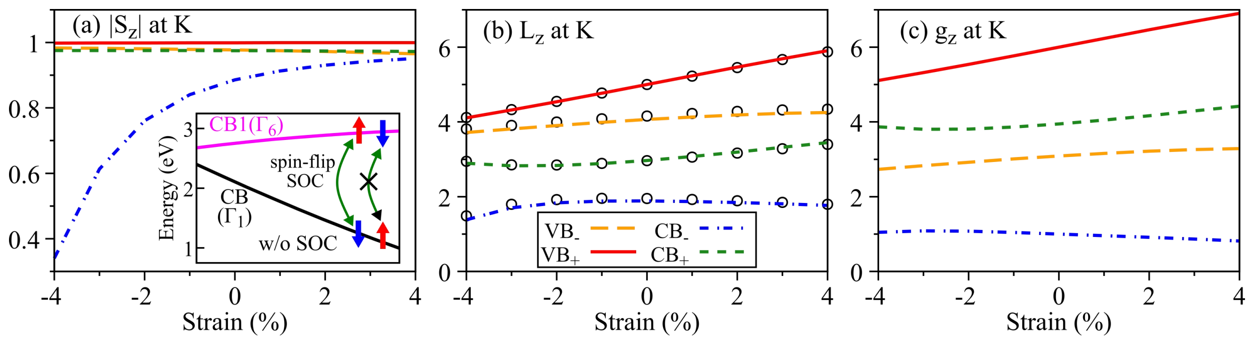

Figure 1: (a) Spin angular momenta, S_z, (b) orbital angular momenta, L_z, and (c) g-factors ($g_z = L_z + S_z$) for the low-energy bands at the K-valley for strained WSe_2 monolayer. The inset in Fig.(a) indicates the microscopic mechanism responsible for the drastic spin mixing in CB-.