

Unveiling elusive physical phenomena in van der Waals systems via the valley Zeeman effect

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The interplay of the spin and the orbital angular momenta of electrons, holes, and their correlated excitonic states, governs the observed Zeeman splitting, which is often described by effective g-factors. In the realm of 2D materials, transition metal dichalcogenides (TMDCs) host robust exciton features and are ideal candidates to explore the manifestation of coupled spin, valley, and orbital degrees of freedom under external magnetic fields. In this talk, I will cover the basic physics behind the valley Zeeman splitting and effective g-factors, emphasizing the recent first-principles developments in monolayer TMDCs that faithfully reproduce the available experimental data[1], offering robust predictive capabilities. These new theoretical insights demystify the valley Zeeman physics in TMDCs and finally establish a connection to the vast existing knowledge in the area of III-V materials. Using this full *ab initio* approach, I will discuss how the spin-valley physics and exciton g-factors can be used to unveil elusive physical phenomena in TMDC-based van der Waals systems. Particularly, I will focus on three different examples: (i) strain effects in monolayer TMDCs[2,3,4], (ii) the valley Zeeman splitting of dipolar excitons in MoSe₂/WSe₂ under external electric field[5], and (iii) the proximity-enhanced valley Zeeman effects in WS₂/graphene systems[6]. These selected examples demonstrate how the microscopic nuances of the valley Zeeman physics reveal elusive physical phenomena in van der Waals materials and heterostructures that are particularly relevant to the fields of valleytronics, straintronics, and twistronics.

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