Excitonic g-factors in van der Waals structures beyond simple models

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The shifts of optical peaks energies under external magnetic field, quantified by effective *g*-factors, provide a deep insight into electronic and excitonic structures of two-dimensional materials. A recently developed first-principles-based method for calculation of *g*-factors, including bands-summation formula, yields excellent agreement with experiments for intralayer excitons in monolayer (1L) transition metal dichalcogenides (TMDCs), interlayer excitons in TMDCs heterobilayers, as well as larger excitonic complexes in doped 1L TMDCs [1,2]. The last case corroborates the accuracy of the method for evaluation of single bands *g*-factors. Here we present more advanced cases which are beyond the possibilities of simplistic models with spin, atomic orbital and valley contributions. We explain the reduction of *g*-factors measured in $MoSe_2/WS_2$ moiré heterobilayer by inclusion of exciton *g*-factor's dispersion and spatial confinement in moiré potential [3]. Inclusion of excitonic wavefunctions calculated by model Bethe-Salpeter equation enables us to understand the measured excitonic state dependence of *g*-factors in 1L and homobilayer TMDCs [4,5]. We analyze the influence of biaxial strain on 1L TMDs, finding a large strain dependence of excitonic *g*-factors, with significant spin-mixing effects [6]. The calculated trends of direct and indirect excitons *g*-factors in WS_2 micro-bubbles allow us to explain the strain-induced exciton hybridization in WS_2 monolayers unveiled by magnetooptical measurements [7]. We investigate a new class of hexagonal 2D materials with formula MSi_2Z_4 (M: Mo, W; Z: N, P, As, Sb), which are isosymmetric to 1L TMDCs. We find a new set of circularly polarized excitonic transitions with high binding energies and large positive g-factors [8].

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