Spin-flip processes and radiative decay of dark intravalley excitons in transition metal dichalcogenide monolayers

A.O.Slobodeniuk D.M.Basko

Laboratoire National des Champs Magnétiques Intenses, CNRS-UJF-UPS-INSA, 25 rue des Martyrs, B.P. 166, 38042 Grenoble, France

artur.slobodeniuk@lncmi.cnrs.frl

Transition metal dichalcogenides (TMDCs) are layered materials with the chemical composition MX₂, where M is a transition metal (such as molybdenum or tungsten), and X is a chalcogen (sulfur, selenium, or tellurium). The interest to semiconducting TMDCs has been sparked by the recent discovery of the monolayer MoS₂ being a direct-gap semiconductor, in contrast to its bulk indirect-gap counterpart. The gap in the visible light range and tightly bound excitons make TMDC monolayers promising for optical applications. There are two types of excitons in such materials: "bright" (which can be created by absorption of light) and "dark" ones (which are formally decoupled from photons). The latter poses a question whether the dark exciton states are optically inactive, or there are some mechanisms for their radiative decay.

We perform a theoretical study of radiative decay of dark intravalley excitons in TMDC monolayers. This decay necessarily involves an electronic spin flip. The intrinsic decay mechanism owing to interband spin-flip dipole moment perpendicular to the plane of the monolayer (mentioned in [1,2]), gives a rate about 100–1000 times smaller than that of bright excitons. However, we found that this mechanism also introduces i) the energy splitting due to a local field effect (which is an analogue of the exchange energy shift of the Z excitons states in semiconductor quantum wells [3,4]); ii) whole oscillator strenath is contained in the higher energy component, whereas the lowest energy state remains dark and needs an extrinsic spin-flip mechanism for the decay. The Rashba effect due to a perpendicular electric field or a dielectric substrate, aives a negligible radiative decay rate (about 10⁷ times less than that of bright excitons). Spin flip process, due to Zeeman effect in a sufficiently strong in-plane magnetic field, can give a decay rate comparable to that owing to the intrinsic interband spin-flip dipole [5].

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