Excitonic properties of transition metal trichalcogenides MPX_3

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Atomically thin, magnetic materials have gained increasing attention since 2017, when the first 2D ferromagnet was reported [1]. This breakthrough has triggered research on 2D magnetic materials [2]. They are not only important from a fundamental point of view -to understand the theory of magnetism in reduced dimensions-, but also for technological applications. However, probing the magnetic order of the 2D systems by conventional magnetic experimental setups is very challenging. On the other hand, it is well known, that even in the single layer limit, semiconducting two-dimensional materials strongly absorb light. Therefore, optical spectroscopy is a good method for their characterization.

In this communication, we present the results of the comprehensive theoretical investigation of the binding energy of the 2D magnetic crystal $MnPS_3$ based on the density functional theory and versatile formalism of the Bethe-Salpeter equation. The $MnPS_3$ is one important example from the large family of transition metal phosphorus trisulfide (MPS_3) [3]. We demonstrate that the large binding energy of the exciton equal to more than 1 eV and obtained for monolayer of $MnPS_3$ [4], is two times greater than in the case of transition metal dichalcogenides. We also highlight the role of the magnetic orderings in electronic and optical properties. In particular, the strong impact of the magnetic ordering on the binding energy of excitons in the monolayer limit is demonstrated, as well as its substantial influence on effective mass of the carriers. In addition, we have shown that the magnetic state of the monolayer samples is sensitive to the polarization of light. Aforementioned results indicate the possibility of indirect probing of magnetic properties via optical or transport measurements.

The study was accomplished thanks to the funds allotted by the National Science Centre, Poland within the framework of the research project ‘SONATA12’ no. UMO-2016/23/D/ST3/03446. Financial support from theDeutsche Forschungsgemeinschaft (DFG, German Re-search Foundation) under Project-ID 314695032 (SFB1277) is acknowledged by P.E.F.J. and J.F. and un-der Project-ID 317551441 by J.K. Access to computing facilities of TU Dresden ZIH for the project ”TransPheMat”, PL-Grid Polish Infrastructure for Supporting Computational Science in the European Research Space, and of the Interdisciplinary Center of Modeling (ICM), University of Warsaw are gratefully acknowledged.

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