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Luis Viña
Departamento de Física de Materiales. C4-507
Universidad Autónoma. Cantoblanco
E-28049 Madrid. SPAIN.
Phone: (34)914974782
Fax: (34)914978579
e-mail: luis.vina@uam.es

Evaluation report of the PhD thesis, entitled “Optical properties of thin layers of transition metal dichalcogenides”, presented by Maciej Koperski to apply for the PhD degree at the University of Warsaw (Poland).

The thesis is well written, with a presentation that makes it easy to read. It is very well structured in three chapters and one Appendix. The illustrations are clear and of high quality and are properly referred to and discussed in the main text of the manuscript.

The student demonstrates a very good knowledge of the state of the art of the subject of his thesis, optical properties of thin films of transition metal dichalcogenides, which is very well presented in the introduction of the different chapters and when it is needed in the discussions of the manuscript. The thesis includes a comprehensive list of references, which are quoted along the different chapters. The collaborations with different groups, especially Polish ones, although not directly mentioned in the manuscript, are evident analyzing the list of publications of the candidate related to his thesis.

The scientific quality of the work is very high: using the appropriate characterization techniques, with well designed, and consciously performed, experiments the student performs a systematic study of the optical properties of these, recently developed, new materials, single- and few-layers of transition metal dichalcogenides. The methodology is adequate and the hypothesis are well validated through the experiments. In some cases, and due to the complexity of the investigated materials, speculations are presented, which, as much as possible, are corroborated by further experiments.

The work is very original, presenting experiments that have not been performed previously in the materials that are investigated. Furthermore, several unpredictable phenomena are discovered in the investigations, which are analyzed with new, phenomenological, models, that had not been considered before in the literature. The classification of the two main types of materials studied into optically “active” and optically “dark” materials, calling for the interpretation that in latter ones the emission arises from excited states is novel. The finding of single-photon emitters, and methods to localize them in the samples, as well as their existence in some samples up to room temperature opens the possibility, with still a large technological development to be realized, to obtain new devices essential for quantum optics and quantum information technologies. It also presents a novel method to identify the number of layers, in a few layer structures, exclusively by analyzing their optical contrast.

The work presents a detailed study of thin films of semiconducting transition metal dichalcogenides, which contributes to the understanding of their electronic properties. The systematic study is made mainly by photoluminescence and reflectivity measurements, as a function of temperature, magnetic field and polarization of the excitation and emitted light, and complemented by scanning tunneling microscope measurements. The effects of the number of layers and temperature on the excitonic resonances in these materials is thoroughly investigated, obtaining important information on the evolution of the band structure with thickness and on the modifications of the Coulomb interaction. A comparison between MoSe₂ and WSe₂ monolayers leads to the conclusion of the existence of two types of spin alignment in the conduction sub-bands. Therefore, optically active excitons are the ground state of MoSe₂, while the existence of lower energy optically inactive dark states is inferred for WSe₂. The magnetic field studies are interpreted based on a simple empirical model, considering three contributions, accounting for spin, orbital and valley-type effects. This model allows the evaluation of the g-factor of an individual electronic state in the conduction band. The appearance of narrow lines emitting centers is analyzed and demonstrated that their emission corresponds to single photons. Their origin is tentatively attributed to the existence of nano-sized monolayers in the case of WSe₂ and to structural defects in the case of boron nitride.

In summary, the thesis presents a thoroughly study on the optical properties of transition metal dichalcogenides, in particular on WSe₂ and MoSe₂ structures. The manuscript is very well structured and written with a proper introduction to the subject and exposition of the state of the art of the knowledge of these materials. The studies yield a classification on “bright” and “dark” materials, depending on the details of their band structure, valley and spin characteristics. Complete, temperature and magnetic field dependent, experiments reveal the different behavior of the materials according to the mentioned classification. Finally, and very importantly, a very detailed study of the single-photon character of the emission in these materials is presented. This study is completed by investigations of boron nitride crystals, which show deep levels that are able to emit single photons up to room temperature.

In my opinion the thesis presented by Mr. Maciej Koperski is very good and solid and certainly sufficient to be the basis for application for a degree of doctor in physics at the University of Warsaw (Poland). Therefore, I am formally requesting that he is permitted to publicly defend it.

Madrid, April 10, 2017



Signed
Luis Viña

Full professor of Condensed Matter Physics
Universidad Autónoma de Madrid (Spain)