CTU
CZECH TECHNICAL UNIVERSITY IN PRAGUE

THESIS REVIEWER'S REPORT

I. IDENTIFICATION DATA

Thesis title:	**Quantum Mechanical study of electronic properties of systems derived from transition metal dichalcogenides**
Author's name:	**Marek Hulec**
Type of thesis :	bachelor
Faculty/Institute:	Faculty of Electrical Engineering (FEE)
Department:	Department of Electromagnetic Field
Thesis reviewer:	Miguel Pruneda
Reviewer's department:	Institut Català de Nanociència i Nanotecnología (ICN2), Barcelona (Spain)

II. EVALUATION OF INDIVIDUAL CRITERIA

Assignment — **ordinarily challenging**

How demanding was the assigned project?

The project is based on first-principles DFT simulations to study the electronic properties of doped few-layer transition metal dichalcogenides. The doping is simulated by substituting the transition metal (Mo or W) by another element (W or Mo, respectively) using a supercell approach. The simulations require familiarity with state-of-the-art computational tools, and a good understanding of the methods and approximations used, although similar studies are available in the scientific literature.

Fulfilment of assignment — **fulfilled**

How well does the thesis fulfil the assigned task? Have the primary goals been achieved? Which assigned tasks have been incompletely covered, and which parts of the thesis are overextended? Justify your answer.

The dependencies of the band gaps with chemical composition, and number of layers in the thin-film have been addressed. Questions for future research have been posed.

Methodology — **correct**

Comment on the correctness of the approach and/or the solution methods.

Overall the methodology used is appropriate. There are however some technicalities that have been avoided. The motivation of the work seems to be related to photovoltaic applications of TMDCs, where in addition to the electronic gap it would have been interesting to address the optical band gap. On the other hand, it is well known that DFT has some problems with the evaluation of the band gap, which have not been discussed in the report. Finally, the supercell used might be too small to simulate the diluted doping concentrations, and the spin-orbit effect (not included in this work) might be important for the tellurides (in particular, for WTe2).

Technical level — **B - very good.**

Is the thesis technically sound? How well did the student employ expertise in the field of his/her field of study? Does the student explain clearly what he/she has done?

The simulations presented are demanding, and require careful analysis. The results are clearly discussed and presented in the report.

Formal and language level, scope of thesis — **A - excellent.**

Are formalisms and notations used properly? Is the thesis organized in a logical way? Is the thesis sufficiently extensive? Is the thesis well-presented? Is the language clear and understandable? Is the English satisfactory?

There is a detailed introduction of the methodology, with the main theory and approximations used in the simulations. The technicalities of the calculations are also well described. If anything, I miss a brief introduction to the pseudopotential approximation, which is used in the work, but not described in the thesis.

Selection of sources, citation correctness — **B - very good.**

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Does the thesis make adequate reference to earlier work on the topic? Was the selection of sources adequate? Is the student's original work clearly distinguished from earlier work in the field? Do the bibliographic citations meet the standards?
Although there are some sentences that seem misunderstanding of the literature, I think the sources and references are adequate. A few examples: 1) in page 3, "Molecular Dynamics" refers to a semiempirical approach for atomistics classical mechanics. However, one can also use "ab initio" MD to include quantum effects; 2) page 4, it is not true that equation 2.7 can only be solved analytically for the hydrogen atom without spin-orbit interaction; 3) page 6, it is not true that the Hartree-Fock method assumes that each electron is moving in a "spherical average"; 4) page 9, the connection between LDA and the compensating uniform positive charge distribution to ensure charge neutrality is either out of context, or wrong; 5) chapter 3: TMDs can have different crystallographic structures, here it seems that only the 2H phase is addressed, although the ditellurides might be stabilized in the T-phase… 6) the reliability of the DFT gaps is not discussed.

Additional commentary and evaluation (optional) *Comment on the overall quality of the thesis, its novelty and its impact on the field, its strengths and weaknesses, the utility of the solution that is presented, the theoretical/formal level, the student's skillfulness, etc.*
I

III. OVERALL EVALUATION, QUESTIONS FOR THE PRESENTATION AND DEFENSE OF THE THESIS, SUGGESTED GRADE

Summarize your opinion on the thesis and explain your final grading. Pose questions that should be answered during the presentation and defense of the student's work.

I think this is a good bachelor thesis, which makes use of advanced simulation methods to address a problem of interest. It poses interesting issues which require careful analysis and thinking on the results. Some of these issues have been addressed, although it seems the student has gone too quickly over others. There are a few questions which I think are important. The first two are related to "materials science" aspects, ant the last ones are more technical.

1) **Why did the student choose these specific dopants? Why not substitutional chalcogenides instead of transition metals? Or why not vacancies?**
2) **The model to describe the doping assumed a supercell 2x2x1. Is this a realistic model? What would be the doping concentration? Would it be achievable experimentally? Furthermore, the dopants would be periodically repeated with this model… plotting the bandstructures (which unfortunately were not presented in the report) would give an idea of the interactions between the dopants.**
3) **The bandstructures were not shown because they gave a band-gap that was smaller than the one computed from the DOS. As explained in the report, this is "surprising" and "unusual" because the k-mesh used for the DOS is smoother than the linear k-path used to plot the bands. What was the k-mesh used in each case? If the bandstructure gives a lower gap, I would trust that value rather than the gap obtained from the DOS…**
4) **Comment on the reliability of the gap in DFT calculations. Which methods could be used to give an improved description.**

The grade that I award for the thesis is **B - very good.**

Date: **19.8.2021**

Signature: