

I. IDENTIFICATION DATA

Thesis title:	Quantum Mechanical Study of Diamond-based Materials for Electronic Applications
Author's name:	Matus Kaintz
Type of thesis :	bachelor
Faculty/Institute:	Faculty of Electrical Engineering (FEE)
Department:	Department of Control Engineering
Thesis reviewer:	Dr. Antonio Cammarata
Reviewer's department:	Department of Control Engineering

II. EVALUATION OF INDIVIDUAL CRITERIA

Assignment	extraordinarily challenging
<i>How demanding was the assigned project?</i>	
The candidate had to learn the fundamentals of Quantum Mechanics and their mathematical formalism; however, the candidate's academic courses did not cover such subjects but he managed to acquire the required knowledge showing extraordinary ability to quickly learn new theories and techniques.	

Fulfilment of assignment	fulfilled
<i>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.</i>	
The thesis had the aim to acquire the necessary knowledge to perform quantum mechanical simulations on solid state systems. The acquired knowledge has been used to study the possible use of diamond for electronic application. The candidate went through both the didactical and the practical aspect of the theme in an excellent way thus fulfilling at the best all the assignments.	

Activity and independence when creating final thesis	A - excellent.
<i>Assess whether the student had a positive approach, whether the time limits were met, whether the conception was regularly consulted and whether the student was well prepared for the consultations. Assess the student's ability to work independently.</i>	
The candidate proposed his own way to extend the planned analysis; his intuitions allowed to uncover some subtle details of the electronic structure which will be subject of further investigation and eventually publication on impacted journals. The high level of his English language allowed him to write the thesis almost independently with limited intervention from my side. The candidate was responding to the assigned task in a timely manner according to the planned schedule.	

Technical level	B - very good.
<i>Is the thesis technically sound? How well did the student employ expertise in his/her field of study? Does the student explain clearly what he/she has done?</i>	
The technical level is high and the results are clearly presented and discussed. For this reason, the results will be part of a planned publication in impacted scientific journals.	

Formal level and language level, scope of thesis	A - excellent.
<i>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?</i>	

The first chapters of the thesis present the quantum mechanical theory and the technical aspects in a way that is a good starting point for all those young investigators at their first approach to the subject. The results are clearly presented in a very fluent English language, easy to understand and technically detailed at the same time.

Selection of sources, citation correctness

B - very good.

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?

The review literature was compiled carefully and includes all the relevant sources. The citations were used correctly.

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.

The candidate faithfully solved the given problem and the achieved results are valuable and add further insight to the knowledge of the physics of the studied system. Considering also that the candidate had to build his own knowledge of the quantum mechanics and the related technicalities and software, I evaluate the whole work as excellent. The candidate is a very promising future independent researcher.

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.

The grade that I award for the thesis is A - excellent.

Date: 17/08/2020

Signature:

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Department:	Department of Control Engineering
Thesis reviewer:	Prof. RNDr. Bohuslav Rezek, Ph.D.
Reviewer's department:	Department of Physics

II. EVALUATION OF INDIVIDUAL CRITERIA

Assignment	extraordinarily challenging
<i>How demanding was the assigned project?</i>	
For bachelor thesis, the assigned project was extraordinarily challenging. The subject demanded to learn a lot of background information including the solid state physics, diamond as semiconductor material as well as about computing methods and actual use of computing software.	

Fulfilment of assignment	fulfilled
<i>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.</i>	
The thesis fulfills the assigned task, i.e. role of dopants/impurities on diamond band gap width and Fermi level position has been theoretically assessed and discussed. The actual validity of the findings still needs to be verified though, including discrepancies with the experimental as well as computational data in the literature (see e.g. doi: 10.1038/nature04278 and 10.1126/science.1172419, 10.1088/0022-3727/42/14/145407)	

Methodology	partially applicable
<i>Comment on the correctness of the approach and/or the solution methods.</i>	
The method of computing doped diamond by DFT has been selected appropriately in general. However, the validity and interpretation of results needs to be discussed. For instance, narrowing of the diamond band gap by such as high amount is hardly realistic. It may rather be that dopants (in particular boron) create additional states in the band gap that are mistaken for conduction band minimum or valence band maximum. Or the computing methods must be improved, see e.g. doi: 10.1088/0022-3727/42/14/145407. Dopant distance to carbon does not seem as a realistic parameter, the system should be rather relaxed and formation energy obtained as indication of incorporation probability. The dopant concentration is also relatively high, actually 0.1 at.% corresponds to about 10^{20} 1/cm ³ doping, 1 at.% is thus already at the metallic transition. Concentration dependence may be thus low. Formation of impurity bands should be considered	

Technical level	B - very good.
<i>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?</i>	
The thesis is written on a technically very good level, considering also particular challenges for the student as described above. The work is described and presented clearly. There are several contradictory statements though, such as that dopants change only the Fermi level vs. they change the band gap.	

Formal and language level, scope of thesis	A - excellent.
<i>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?</i>	
On a formal level, the thesis is also well prepared and organized. The text is well readable, including quality of English. Figures are well prepared, they have publication quality. Only most of the figure is placed after the discussion part rather than in the results section. For the bachelor thesis it is sufficiently extensive. For instance, the student was employing 5 types of impurity atoms (providing donor or acceptor levels) and 3 levels of concentrations for each.	

Selection of sources, citation correctness**C - good.**

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?

The thesis provides reasonable references to prior works and fundamental textbook information. Selection of sources is somewhat peculiar though, in particular in diamond they rather out of the mainstream. Some of the key relevant works are missing and actually considering them would make the thesis more relevant and valid. Student's own work is clearly distinguished from prior works. Yet it should be mentioned during the defense what he has done himself (maybe all, but it is not mentioned).

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.

The thesis presents an interesting idea of diamond band gap width modification by dopants. It is generally possible (see e.g. 10.1126/science.1172419) but the presented amount of change is not realistic. Thus, the methodology and interpretation of results still need careful consideration. It should be also more correlated with available experiments and computational results in the literature on diamond. Yet let me say that as bachelor thesis it was indeed extraordinarily challenging topic to master. The student made reasonable effort to tackle this subject.

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.

The thesis presents an interesting idea of diamond band gap width modification by dopants. The methodology and interpretation of results still need careful consideration and correlation with the available literature on diamond. Nevertheless, as bachelor thesis it was indeed extraordinarily challenging topic to master. The student made reasonable effort to tackle this subject. Technically the thesis was well prepared.

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

Date: 20.8.2020

Signature: