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Faculty  
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Jihočeská univerzita  
v Českých Budějovicích  
University of South Bohemia  
in České Budějovice

## OPPONENT'S REVIEW ON BACHELOR THESIS

**Name of the student:** Marc Ninou Codina

**Thesis title:** Theoretical study of bacteriochlorophyll aggregates using methods of quantum chemistry and molecular mechanics

**Supervisor:** Mgr. David Řeha, Ph.D.

**Referee:** MSc. Denys Biriukov

**Referee's affiliation:** University of South Bohemia, Faculty of Science, Institute of Physics

	Point scale	Points
<b>(1) FORMAL REQUIREMENTS</b>		
<b>Extent of the thesis</b> (for bachelor theses min. 18 pages, for masters theses min. 25 pages), <b>balanced length of the thesis parts</b> (recommended length of the theoretical part is max. 1/3 of the total length), <b>logical structure of the thesis</b>	0-3	3
<b>Quality of the theoretical part (review)</b> (number and relevancy of the references, recency of the references)	0-3	3
<b>Accuracy in citing of the references</b> (presence of uncited sources, uniform style of the references, use of correct journal titles and abbreviations)	0-3	3
<b>Graphic layout of the text and of the figures/tables</b>	0-3	3
<b>Quality of the annotation</b>	0-3	3
<b>Language and stylistics, complying with the valid terminology</b>	0-3	2
<b>Accuracy and completeness of figures/tables legends</b> (clarity without reading the rest of the text, explanation of the symbols and labeling, indication of the units)	0-3	3
<b>Formal requirements – points in total</b>		20
<b>(2) PRACTICAL REQUIREMENTS</b>		
<b>Clarity and fulfillment of the aims</b>	0-3	3
<b>Ability to understand the results, their interpretation, and clarity of the results, discussion, and conclusions</b>	0-3	3
<b>Discussion quality – interpretation of the results and their discussion with the literature</b> (absence of discussion with the literature is not acceptable)	0-3	2
<b>Logic in the course of the experimental work</b>	0-3	3
<b>Completeness of the description of the used techniques</b>	0-3	3
<b>Experimental difficulty of the thesis, independence in experimental work</b>	0-3	3

Quality of experimental data presentation	0-3	3
The use of up-to-date techniques	0-3	3
Contribution of the thesis to the knowledge in the field and possibility to publish the results (after eventual supplementary experiments)	0-3	3
Practical requirements – points in total		26
<b>POINTS IN TOTAL (MAX/AWARDED)</b>	<b>48</b>	<b>46</b>

### **Comments of the reviewer on the student and the thesis:**

In his bachelor thesis, Marc Ninou Codina investigates the molecular origin of the self-assembly of BChl aggregates into higher-order structures using computational methods. Particularly, this study aimed to check the hypothesis whether the curvature formation of those aggregates is dictated by local interactions and stabilization of BChl molecules in a single aggregate, particularly a tetramer, or there should be another explanation for such self-organization. This research can substantially help in understanding, which molecular mechanisms are in charge for such self-composition, and what is their role in related light harvesting reactions, with possible future applications of these findings in nano and energy technologies.

The thesis employs QM/MM methods that have been proven a powerful tool in addressing such type of speculations due to an adequate compromise between accuracy and required computational power. The methodology is comprehensible and well-written, results are clearly summarized, and lead to a straightforward conclusion that local interactions are not responsible for self-organization, and rather entropic or macromolecular effects may play a key role. Some parts and especially some statements in the results and discussion are not entirely accurate or even needed (e.g. on p.28 the Symmetry Adapted Perturbation Theory is too detailed, so might be either shortened and moved to the Methods or completely deleted), however this does not erode the value of the scientific outputs. The discussion and comparison with available literature data are present, and possible outlines for the future work are drawn and give food for thought.

Overall, the impression from the thesis is very positive, especially as for a bachelor work. Obtained results can easily give a try being published in an international peer-reviewed journal, if additional more accurate calculations, e.g., using already tested MP2 method, will be added and discussed. The student made an excellent work, and therefore his thesis deserves the grade “excellent”.

### **Mistakes, which the students should avoid in the future:**

1. There are few places with weird formulations or obvious typos (e.g. the top of p.12 and bottom of p.16).
2. The discussion of energy differences is a bit harsh. On p.31 the student wrote that DFT calculations overestimate the interaction energy by 10 kcal/mol, when compared to the MP2 method. Actually, the overestimation is nearly 16 kcal/mol, and neglecting 6 kcal/mol devalues some conclusions based on the results in Tables 1-3, where the difference in 6-8 kcal/mol is treated as that tetramers are “clearly stabilized” in one pattern with respect to another.

**Suggestions and questions, to which the student has to answer during the defense:**

1. What is BChl f? Its structure is shown in Figure 4, however nothing is written about its nature.
2. What do “d” and “dd” stand for in namings like “ $\alpha S\beta A$ -dd”? It is not mentioned in the corresponding paragraph on p.20.
3. One single calculation performed using the MP2 method hardly provides any new valuable information. This calculation confirms neither difference between  $\beta A\beta A$  and  $\alpha S\beta A$ -dd tetramers nor trends in interaction energies depending on the location of a tetramer. Is there a hope that additional results (or at least some preliminary data) using the MP2 method will be obtained prior to the defense?
4. What are estimated errors in energy calculations from DFT? Is the 6 kcal/mol difference (Table 1, the  $\alpha S\beta A$ -dd case) large enough to draw further conclusions?
5. It would be better if Figure 15 provided a few more views from other sides on the compared tetramers. It would improve the visualization and highlight differences in the geometry of the structures.

**Conclusion:**

In conclusion, I

r e c o m m e n d

the thesis for the defense and I suggest the grade **excellent** .

In **Ceske Budejovice** date **22th January 2020**

  
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signature