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Doctoral thesis “Electronic Structure Effects in Molecular Junctions” by Mr Štěpán Marek

To whom it may concern,

As appointed referee by the Faculty of Mathemathics and Physics, Charles University, I have the honour to evaluate the PhD thesis titled "Electronic structure effects in molecular junctions" by Mr Štěpán Marek. This evaluation assesses the novel scientific contributions of the thesis, its significance within the field of molecular electronics, and the candidate's demonstration of creative scientific inquiry.

Overview of the thesis:

The candidate's work ambitiously explores the fundamental aspects of molecular electronics, emphasizing the critical role of numerical tools and effective models in understanding quantum transport phenomena. The thesis is structured around three pivotal studies: the investigation of elastic transport in ferrocene molecular junctions, the examination of electronic momentum transfer in helical molecules, and the application of the GW approximation in finite-sized metallic clusters. This approach provides a comprehensive insight into the complex interplay between atomic/molecular structure and electronic properties.

Evaluation of individual chapters:

Chapter 1 successfully outlines the research scope and introduces the field of molecular electronics, setting a solid foundation for the subsequent investigations. However, more detailed background and motivation for the chosen research topics could enhance the reader's understanding of their significance.

Chapter 2 is notable for its original theoretical contributions, particularly some innovative aspects of a derivation of the current formula and related operators. A clearer exposition of these theoretical developments in term of their practical implementations would further strengthen this chapter. A link to the established concept of “bond currents” could have been interesting.

Chapter 3, while concise, could benefit from a more detailed discussion on the selection of methodologies and their impact on the research outcomes. For instance, the so-called “ev-GW” method is only briefly outlined although this is not

a completely standard approach.

Chapter 4 presents the core findings of the thesis. The exploration of geometric aspects of ferrocene molecular junctions, of electronic currents through helical molecules inducing angular momentum transfer, and of correlation effects in the energy spectrum of sodium clusters introduces novel insights into molecular electronics. Each study contributes to the field, though a more explicit statement of conclusions and implications would be valuable.

General observations:

Mr Štěpán Marek's thesis is a testament to his dedication and innovative approach to understanding electronic structure effects in molecular junctions. It presents several original ideas that contribute meaningfully to the field. Nonetheless, the thesis would have benefited from more critical proofreading. Enhancing the clarity of presentation and addressing typographical errors would significantly improve its readability and educational value. I recommend that Mr Štěpán Marek take this as encouragement to continue refining his approach to scientific writing and presentation.

Conclusions and recommendations:

The thesis demonstrates Mr Štěpán Marek's ability to engage in creative and significant scientific research, contributing new knowledge to the field of molecular electronics.

At the defense, a dialogue around the following areas could be beneficial:

- Experimental findings that motivate this work,
- Discussion on methodological choices and their implications,
- Exploration of future research avenues, especially regarding the novel findings on angular momentum transfer.

In summary, I commend Mr Štěpán Marek for his work and look forward to good discussions at the defense as well as to his future contributions to the scientific community. I particularly encourage him to pursue publication of his findings on angular momentum transfer in the helical molecules, an area that represents a significant opportunity for advancing the field.

Sincerely,

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