Reviewer report to the PhD thesis entitled *"2D Materials for Solar Energy Conversion"*
by
Mgr. Jaroslava Ňáhová

The submitted PhD thesis of Mgr. Jaroslava Ňáhová is a well-executed investigation into the effects of substrate types and the mechanical and optoelectronic properties of two-dimensional (2D) materials, particularly graphene and transition metal dichalcogenides (TMDCs), for solar energy conversion. The work provides valuable insights into how substrate interactions and mechanical strain can tune these properties, advancing photovoltaic technologies.

The thesis consists of three main parts. The initial two parts introduce the 2D materials, their phonon characteristics, and the principle of atomic force microscopy techniques using the different modes. The thesis topic and content are relevant to the research area, and the approach and methods used are appropriate. The third part of the PhD thesis is dedicated to discussing and interpreting the research findings. It is divided into five main groups, focusing on the photovoltaic properties of graphene-silicon, graphene wrinkling, and wrinklons, interactions in Au-TMCD, and the concept of energy funneling in WSe_2.

The thesis investigates the mechanical and optoelectronic properties of two-dimensional (2D) materials, specifically graphene, and TMDCs, and their applications in solar energy conversion. By focusing on how these properties can be tuned through substrate interaction and mechanical strain, the study contributes to advancing photovoltaic technologies. It employs advanced characterization techniques such as Atomic Force Microscopy (AFM) and Raman Spectroscopy to elucidate these mechanisms, providing important information for future innovations in 2D material-based devices.

The formal appearance and level of the PhD thesis are of high quality. The PhD thesis is well-structured, with 75 pages including 34 Figures, 2 Tables, and 160 literature resources, and well-written in English. The results are described, argued, and compared with relevant literature in a manner that reflects deep understanding and engagement with the topic.

The PhD thesis contains many original results discussed in great detail, well described, well-argued, and compared with relevant published literature. A large part of the results came from PhD thesis of Mgr. Jaroslava Ňáhová led to scientific outcomes published in good-designated internationally impacted journals, wherein one of them, Mgr. Jaroslava Ňáhová is the first author and for three of them, as a co-author with a significant contribution. To conclude, the findings obtained within the PhD thesis of Mgr. J. Ňáhová are novel and will provide significant knowledge in the research field area.

I have found only a few minor inconsistencies thorough reading the text (SPM shortcut introduced later than first appearance, inconsistency in c-AFM and C-AFM, meaning of 1L is not introduced, etc). These issues, however, are relevant to the quality of the research presented.

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In the end, I would appreciate a more detailed discussion on the following topics during the PhD defense:

1. In Figure 3.6, the PL spectra of 1L free TMDC show prominent peaks around 600 – 800 nm (depending on TMDC), which are not discussed in the text. What transitions do these peaks correspond to, and how do they relate to the material's band structure?

2. Why was a gold-coated substrate selected for exfoliation experiments instead of other metals, such as platinum, which might exhibit similar behavior?

3. In many cases, the 2D materials were prepared by mechanical exfoliation. As mechanical exfoliation is tricky, how well is the synthesis reproducible?

    a. Did you conduct statistical studies to assess property deviations between samples?
    b. What strategies were implemented to ensure reliable and reproducible results?

4. Presented AFM topography in Figure 3.2 A was done in which mode?

5. Why was only Raman spectroscopy employed for interaction studies? Did you consider some other more suitable techniques for studying interactions?

Jaroslava's PhD thesis meets all the requirements for the degree, and I wholeheartedly recommend awarding Jaroslava with a well-deserved Ph.D. degree after her successful defense.

in Prague 9.12.2024

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