Wrocław University
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Opinion about doctoral thesis of **Madame Amina LAOUID**

Thesis title: **Nanostructures and thin films of metal-organics complexes and hybrid perovskites for applications in optoelectronics and photovoltaics.**

Doctoral thesis of Madame Amina LAOUID has been done under supervision of Prof. Professor **Anna Zawadzka** and Professor **Amine Alaoui Belghiti.** The thesis presents an impressive body of interdisciplinary research that combines experimental and theoretical approaches, to address key challenges in contemporary physics, materials science and sustainable energy technologies. The work was conducted as part of an international cotutelle program between Nicolaus Copernicus University in Toruń, Poland, and Chouaib Doukkali University in El Jadida, Morocco.

The dissertation adopts a cumulative structure, incorporating six original scientific publications that have been peer-reviewed and published in reputable international journals (e.g., Vacuum, Optical Materials, Solar Energy Materials and Solar Cells, Materials Science and Engineering: B). These publications collectively explore the synthesis, structural and morphological characterization, and optoelectronic behavior of functional thin-film materials—namely metal-organic complexes (such as Znq_2:DCM systems) and both organic-inorganic and lead-free perovskite materials. The research is framed around relevant technological goals: improving the performance, stability, and sustainability of materials for photovoltaic and optoelectronic applications.

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One of the key strengths of this dissertation is its comprehensive methodological framework. The candidate combines material fabrication via physical vapor deposition (PVD) with extensive experimental characterization techniques, including atomic force microscopy (AFM), scanning electron microscopy (SEM), UV-Vis spectroscopy, Fourier-transform infrared spectroscopy (FTIR), steady-state and time-resolved photoluminescence (PL), and X-ray fluorescence (XRF). These are complemented by numerical modeling approaches: density functional theory (DFT) calculations to probe electronic structure, and SCAPS-1D simulations to assess photovoltaic device behavior.

This integration of experimental and theoretical methods is skillfully executed. For instance, in the case of the Znq_2:DCM thin films, the candidate investigates energy transfer mechanisms via Förster resonance and validates photophysical interpretations using both PL spectroscopy and DFT-based HOMO-LUMO calculations. In studies of lead-free perovskite materials, such as RbSn0.5Ge0.5I3, the candidate not only characterizes the materials structurally and optically but also models the device-level performance under different architectural configurations, identifying optimal layer combinations and doping levels to improve efficiency and reduce toxicity.

The quality and originality of the scientific content are evident. The candidate's studies on second- and third-order nonlinear optical (NLO) properties in Znq_2-based systems are of particular interest, as they reveal significant potential for applications in nonlinear photonics and signal processing. The dissertation also contributes to the emerging field of environmentally sustainable photovoltaics by evaluating the properties of low-toxicity perovskite formulations under varying temperature and pressure conditions—relevant not only for terrestrial use but also for space applications, as suggested by the experimental studies conducted at cryogenic temperatures.

Importantly, the candidate's personal contribution is substantial. She is listed as the first author on five of the six included articles, with declared contributions ranging from 50% to over 60%. These contributions encompass the entire research

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process, from conceptualization and experimental design, through laboratory work and data analysis, to manuscript drafting and revision. The independence and research maturity demonstrated are appropriate for the level of a doctoral degree and indicate readiness for continued research or academic leadership.

Despite the many strengths of this work, a few critical remarks should be noted to provide a balanced assessment. **Firstly,** although the cumulative format is acceptable, the thesis lacks a fully integrated, comparative discussion that synthesizes the findings of the individual papers into a unified scientific narrative. A dedicated "Discussion" or "Synthesis of Results" chapter could help elucidate the overarching contributions of the work, draw connections between seemingly independent experiments, and reflect more deeply on the broader scientific and technological implications.

Secondly, while the modeling efforts using SCAPS-1D and DFT are valuable, they would benefit from greater methodological transparency. In particular, the SCAPS simulations would be significantly strengthened by a more detailed justification of input parameters, sensitivity analyses, and experimental validation of model assumptions. The DFT calculations, while well presented, could benefit from benchmarking with different functional/basis sets or comparison to alternative electronic structure methods to increase their robustness.

Thirdly, some points requiring clarification, e. g. what was the rationale behind choosing specific doping levels and materials (e.g., Znq2, DCM)? Were these based on prior theoretical predictions or empirical optimization? Why was Znq2 selected as a host material for NLO studies, and how does its performance compare with other known materials such as Alq3? Stability studies are missing, particularly for perovskites. What is the performance under prolonged illumination, humidity, or temperature cycling?

Lastly, some aspects of the experimental data presentation could be improved. For example, the results of morphological measurements (AFM, SEM) are presented descriptively, but lack statistical quantification (e.g., roughness distributions, standard deviations) that would increase scientific rigor. Similarly, although UV-Vis

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and PL spectra are interpreted competently, the connection to material structure (e.g., phase purity, molecular packing) could be explored further using techniques such as X-ray diffraction or XPS, which were not included.

Despite these relatively minor shortcomings, the dissertation as a whole demonstrates a high level of scientific originality, technical competence, and relevance to current and emerging challenges in optoelectronics and photovoltaics. The candidate has produced significant and novel results, disseminated them through high-quality publications, and demonstrated the ability to conduct independent and innovative research of international standing.

Concluding I can say, that **Madame Amina LAOUID** is an expert in investigation of advanced materials for optoelectronic and photovoltaic applications. She is a co-author of 13 publications which recently appeared in highly ranked journals. In ISI Web of Knowledge one can find that his papers already have been cited 54 times, moreover she reported her results on 9 international scientific conferences. I consider that the dissertation meets, and in several aspects exceeds, the formal and substantive requirements for the award of the academic degree of Doctor of Physics. **I therefore strongly support the acceptance of this dissertation.**

At the same time, **I recommend that the doctoral degree be awarded with distinction** based on the following justification: the doctoral thesis by Amina Laouid presents a highly original and scientifically significant body of research in the field of optoelectronics and photovoltaics. The work combines experimental and theoretical investigations on thin films and nanostructures of metal-organic complexes and hybrid perovskites—materials of great relevance for next-generation energy devices. The originality of the dissertation lies in the integrated use of advanced physical vapor deposition (PVD) techniques, nonlinear optical characterization (e.g., second- and third-harmonic generation), and comprehensive theoretical modeling via SCAPS and density functional theory (DFT). Such a combination of methods is rarely applied so cohesively and effectively in doctoral-

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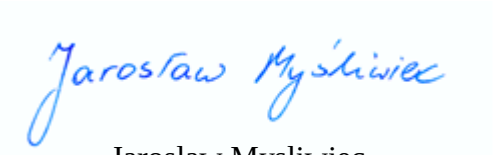
level research. The thesis has also resulted in six peer-reviewed publications, five of which list the candidate as the first author and have been published in reputable journals indexed with significant ministerial (MN) point values and impact factors: 70 pts (Vacuum, Optical Materials, Materials Chemistry and Physics), 100 pts (Environmental Science and Pollution Research, Materials Science & Engineering B), and 140 pts (Solar Energy Materials and Solar Cells).

This is a testament to both the scientific value and the innovation of the work. In light of these contributions, the dissertation clearly stands out in terms of originality and scientific impact and merits **distinction**.



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