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Prof. dr Miljan Bigović

Poštovani profesore Bigoviću,

U prilogu akta vraćamo Vam doktorsku disertaciju doktoranda mr **Božidara Šoškića** pod naslovom: **„Magnetism and superconductivity in two-dimensional (2D) boron crystal structures“** i Izvještaj o ocjeni doktorske disertacije koji su u skladu sa članom 42 stav 3 Pravila doktorskih studija dostavljeni **Centralnoj univerzitetskoj bibliotec** 14. 05. 2025. godine na uvid i ocjenu javnosti.

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PhD jury report of the doctoral thesis

"MAGNETISM AND SUPERCONDUCTIVITY IN TWO-DIMENSIONAL (2D) BORON CRYSTAL STRUCTURES"

written by candidate: Božidar Šoškić (02/2018)

University of Montenegro & University of Antwerp

1. *Dissertation Overview (Bibliographic Information and Summary)*

The primary research area of this doctoral dissertation lies within the field of condensed matter physics, with a specific focus on the exploration of magnetism and superconductivity in two-dimensional (2D) boron crystal structures, commonly referred to as *borophenes*. These materials have attracted significant scientific interest due to their exceptional physical properties, including high electrical conductivity, robust mechanical strength, intrinsic metallicity, and the potential to host superconductivity. Such characteristics establish borophenes as strong contenders among elemental 2D materials, potentially surpassing graphene in advanced electronic and superconducting applications.

Despite their theoretical promise, most of borophenes' remarkable properties remain unconfirmed experimentally. Furthermore, their synthesis remains challenging, requiring specific substrates and tightly controlled growth conditions. Borophene synthesis is often hindered by the presence of impurities, limited scalability, and most critically, a high susceptibility to oxidation. To address these issues, this work investigates novel borophene-based configurations, such as hydrogenated and bilayer structures, that exhibit enhanced resistance to oxidation. Therefore, the central focus of the dissertation is on exploring these systems as potential platforms for stabilizing artificial 2D magnets and their potential for hosting phonon-mediated superconductivity.

To provide a clear understanding of the complexity of the research problem, this dissertation is organized into five chapters, emphasizing core concepts, offering a comprehensive overview of the study, used methodology and presenting key results alongside well-supported conclusions and clearly defined scientific contributions. Before delving deeper into the core of the research, the reader is first provided with a short overview through the abstract, presented in three languages – English, Montenegrin (in extended form), and Dutch – in accordance with the joint PhD agreement between the University of Montenegro and the University of Antwerp. The final section of the dissertation includes the candidate's curriculum vitae, bibliography, and the standard declarations required for submission.

A summary of each **chapter** follows, highlighting the key concepts and findings.

Chapter 1 introduces the field of 2D materials, beginning with an overview of their significance and followed by a focused discussion on borophenes.

The *section 1.1.1* underscores the transformative discovery of graphene in 2004, the 2D allotrope of carbon, whose physical properties surpass those of conventional three-dimensional (3D) materials in complexity and intrigue. This discovery opened the way for the exploration and fabrication of various non-carbon-based 2D materials, including materials from graphene-family and other potential elemental 2D materials – each composed of a single type of atom. Given the diversity of available methods of their synthesis *Section 1.1.2* aim to provide a comprehensive description of the main techniques for their fabrication. *Section 1.1.3* examines the importance of various characterization techniques and their role in refining and optimizing the fabrication of 2D materials for practical applications. On top of that, integrating 2D materials into electronic and optoelectronic devices introduces significant challenges, primarily due to the stringent conditions required for their growth, transfer, and integration. *Section 1.1.4* highlights the key transfer techniques and discusses their importance in enabling the "real-world" application of 2D materials in advanced technological devices. Techniques such as photolithography, electron beam lithography, and nanoimprinting provide fine control over the material's shape and feature size, which is crucial for the development of high-performance electronic and optoelectronic devices. *Section 1.1.5* explores these patterning methods in detail, emphasizing their significance in advancing device fabrication technologies and improving device performance by enabling the precise control of material application in a wide range of fields, including electronics, optoelectronics, sensing, and energy devices. *Section 1.1.6* provides an in-depth exploration of the post-transfer techniques, highlighting their potential to enhance the functionality of 2D materials and unlock new possibilities for cutting-edge technological innovations.

Section 1.2.1 offers a concise yet insightful historical overview of elemental boron, tracing the path from its early use in the form of borate minerals to the theoretical prediction and subsequent investigation of 2D boron sheets – borophenes. Then, the *Section 1.2.2* provides a comprehensive analysis of current borophenes synthesis methods and their characterization, highlighting the crucial "link" between experimental techniques and theoretical modeling via density functional theory (DFT). In the *Section 1.2.3* the author provides a comprehensive overview of borophene's physical properties, highlighting its tunable mechanical, electronic, thermal, and optical characteristics.

Chapter 2 outlines the methodologies employed in the exploration of the magnetic and superconducting properties of both bare and functionalized borophenes, primarily based on first-principles calculations using DFT and its extensions like spin-dependent DFT (SDFT) and density functional perturbation theory (DFPT). *Section 2.1* provides a concise introduction to DFT as a quantum mechanical framework for modeling ground-state properties of materials based on electron density as main variable instead of complex wave functions. *Section 2.2* extends the DFT framework to magnetic systems by explicitly incorporating spin degrees of freedom. Furthermore, the inclusion of relativistic effects, particularly spin-orbit coupling (SOC), is essential for accurately capturing magnetic anisotropy and emergent spin-related phenomena. This formalism provides the foundation for computing magnetic ground states, exchange interactions, and spin textures in complex materials. *Section 2.3* builds on the SDFT formalism to explore the microscopic origins of magnetism in materials, focusing on the fundamental mechanisms that drive magnetic ordering. *Section 2.4* introduces density functional perturbation theory (DFPT) as a key extension of DFT that enables calculation of phonon frequencies via second derivatives of the total energy. DFPT also provides a rigorous route to extract electron-phonon (*e-ph*) coupling matrix elements, essential for understanding superconductivity. *Section 2.5* presents the theoretical foundations of superconductivity, emphasizing its phonon-mediated mechanism and the methodologies used to model it from first principles.

In ***Chapter 3,*** the magnetic properties of two classes of borophene-based systems are investigated: Fe nanostructures adsorbed on β_{12} borophene supported by an Ag(111) substrate, and metal-intercalated bilayer borophene. *Section 3.1* explores the magnetic behavior of Fe nanostructures on β_{12} borophene supported by an Ag(111) substrate, using SDFT and spin model analysis. On the other hand, *Section 3.2* focuses on *3d* metal-intercalated bilayer β_{12} borophene, specifically Mn as intercalant which is identified as the only dynamically stable configuration that retains a finite magnetic moment.

Chapter 4 focuses on the superconducting properties of boron-based 2D materials, with particular emphasis on bare β_{12} borophene, its hydrogenated configurations, and metal-intercalated bilayer structures. Contrary to earlier theoretical predictions suggesting intrinsic superconductivity in freestanding β_{12} borophene, the study described in Section 4.1 reveals that the bare monolayer is dynamically unstable unless it is stabilized by biaxial tensile strain – typically induced by a substrate. Hydrogenation of β_{12} borophene significantly improves both structural stability and superconducting behavior. By tuning strain conditions and carrier concentrations (hole doping), the anisotropic critical temperatures (T_C) up to 30 K are achieved showing also a single-gap nature of this system. These results offer a realistic route for experimental exploration, especially given recent progress in transferring borophene to non-metallic substrates. Beyond monolayers, the study extends – in *section 4.2* – to intercalated bilayer β_{12}, χ_3, δ_4, and kagome borophene phases. A systematic screening of intercalants – including alkali, alkaline-earth, and transition metals – leads to the identification of 17 stable superconducting candidates. Altogether, this chapter establishes borophene-based materials as a highly versatile platform for engineering high-T_C superconductors in low dimensions, with promising implications for nanoelectronic and quantum device applications.

Finally, the main conclusions of the work are summarized in ***Chapter 5***.

2. Dissertation Evaluation

2.1. Problem (state unresolved and controversial opinions about the research problem and previous attempts to solve the problem, solutions reached by other authors, assessment of the dissertation basis in accordance with the publications and research of the candidate and the way they relate to the dissertation)

While intrinsically non-magnetic, bare borophene can exhibit spin-polarized behavior through defect formation or transition metal doping, without the clustering as typically seen in graphene. Initial studies have shown that single- and double-vacancy configurations in β_{12} and χ_3 borophene can induce local magnetic moments; however, these are generally weak (<0.5-1 μ_B) and highly sensitive to the vacancy geometry and carrier concentration. Despite demonstrating the possibility of long-range ferromagnetic coupling via itinerant *p* orbitals and RKKY-like interactions, such defect-engineered magnetism remains limited by its fragile nature and lack of tunability. Furthermore, prior efforts involving non-metallic substitution (e.g., H, N, C) largely failed to enhance or stabilize the magnetic behavior. Transition metal doping, while more promising – especially with 3*d* elements such as Cr, Mn, and Fe – has largely focused on stability, binding nature and spin moments without fully addressing the microscopic origins of exchange interactions. The dissertation effectively identifies this "gap" and advances the field by moving beyond phenomenological descriptions, employing advanced first-principles methods to unravel the fundamental mechanisms of magnetic

ordering. This work thereby establishes a critical theoretical foundation for future exploration of engineered magnetism in 2D boron-based systems.

Furthermore, according to BCS theory, materials composed of light elements are "natural" candidates for high-temperature superconductivity due to their stronger *e-ph* coupling. While most 2D materials like graphene, silicene, and phosphorene require external modifications – such as doping or strain – to induce weak superconductivity, borophene stands out due to its intrinsic metallicity and strong theoretically predicted electron-phonon coupling. Earlier first-principles studies predicted moderate T_C values (12–24 K) for β_{12} and χ_3 phases; however, these models often relied on idealized, freestanding structures later shown to be dynamically unstable. Experimental validation remains limited: Raman-based estimates yield significantly lower T_C values (7–10 K), and no direct superconducting signature has been observed to date. This thesis revisits the problem from a first-principles perspective, showing that bare β_{12} borophene is dynamically stable only under strain, but without traces of superconducting behavior. Furthermore, it is shown that hydrogenation does enhance T_C values in contrast to previous reports, while strain and hole doping can further enhance the T_C up to 30 K. A comprehensive anisotropic Migdal-Eliashberg analysis across various bilayer configurations reveals that superconductivity in borophene is highly sensitive to the orbital composition at the Fermi level, with intercalated bilayers such as Ca–kagome systems emerging as the most promising, reaching T_C up to 58 K. These findings clarify inconsistencies in the literature and define realistic pathways for future experimental exploration.

2.2. Goals and hypotheses of the dissertation

The central goals and working hypotheses of this thesis can be effectively articulated through the following guiding research questions:

1. *Given its pronounced chemical reactivity and the regular arrangement of hexagonal voids, does borophene have the potential to serve as an ideal platform for the adsorption, formation, and stabilization of artificial 2D magnetic structures?*
2. *If so, can such an intercalated 2D magnetic system be formed and stabilized within bilayer borophene, considering that these configurations are more resistant to oxidation and thus offer greater potential for practical applications in spintronics?*
3. *Although previous studies have suggested that bare β_{12} borophene is an intrinsic superconductor, experimental confirmation remains elusive. This raises a critical question: are the earlier theoretical models truly reliable, and can hydrogenation contribute to both the stabilization and protection of this structure against oxidation?*
4. *Finally, can intercalation in bilayer forms of various borophene phases lead to the discovery of an ideal candidate for superconductivity?*

2.3. Essential methods applied in the dissertation and their suitability. If a new or amended method has been applied, describe what is new

The data presented in this work were obtained through first-principles calculations based on DFT, employing a suite of state-of-the-art computational packages, including Quantum ESPRESSO, VASP, Wien2k, GPAW, Phonopy, Wannier90, and EPW.

For the study of magnetism, SDFT calculations were performed, including **constrained non-collinear spin** calculations, to calculate exchange parameters. The primary electronic structure calculations were carried out using **VASP**, **Quantum ESPRESSO**, and **Wien2k**, depending on the symmetry and numerical requirements of the system. Subsequently, **maximally localized Wannier functions** were constructed via **Wannier90 code**, enabling an accurate mapping of *ab initio* results onto localized basis sets. Magnetic exchange interactions were extracted through two complementary approaches: the **four-state method (4SM)** and the **TB2J** code, which uses Green's function formalism and Wannier-based tight-binding models to compute isotropic and anisotropic exchange tensors. A novel methodological approach used in this thesis is the **Successive Hopping Inclusion Method (SHIM)**, to resolve the microscopic origin of magnetic exchange interactions. While previous studies relied primarily on schematic representations of superexchange mechanism, often treating multiple exchange channels collectively and qualitatively, SHIM provides a systematic and quantitative framework. The method progressively includes hopping paths between different orbitals by gradually lowering the hopping parameter threshold $\tau<|t|$, allowing the disentanglement of individual exchange paths in an orbitally resolved basis. This approach enables the identification and isolation of specific hopping path responsible for microscopic magnetic mechanisms – such as direct exchange, superexchange, or super-superexchange – that contribute to the total magnetic coupling, representing a significant advancement over conventional, undifferentiated analyses. Finally, the extracted terms of Heisenberg Hamiltonian were then used as input for **classical Monte Carlo simulations** to estimate thermodynamic properties such as the Curie temperature and magnetic phase stability.

For superconductivity, the methodology combines ground-state DFT calculations with **DFPT** to obtain phonon dispersions and electron-phonon coupling (EPC) matrices. These were calculated primarily using **Quantum ESPRESSO** and post-processed through **EPW** (Electron-Phonon Wannier), which leverages Wannier interpolation to achieve high-resolution EPC data on dense **k/q** meshes. Initial estimates of the superconducting critical temperature (T_C) were obtained using the **McMillan–Allen–Dynes (MAD)** formula under the isotropic approximation. To capture the anisotropic and multi-gap nature of superconductivity in borophene systems, the **fully anisotropic Migdal–Eliashberg equations** were solved using EPW, allowing for a detailed understanding of momentum-resolved gap functions and the orbital character of the pairing mechanism. On top of that, this thesis introduces several methodological advancements to improve the reliability and physical accuracy of superconductivity-related simulations in 2D boron-based materials. First, to capture the effects of electrostatic gating, a field-effect transistor (FET) configuration was implemented using a planar electrostatic potential barrier in the vacuum region, enabling more realistic non-uniform charge doping of the considered systems. Second, instead of using standard-basic acoustic sum rule (ASR) for IFCs in this thesis Born-Huang invariance conditions are implemented, enforcing translational and rotational symmetry to ensure correct low-**q** behavior of flexural phonons, which are essential in 2D systems. This correction, allowed for more accurate prediction of dynamical stability under higher doping levels (up to 0.12 e/B), compared to the limit of 0.03 e/B using only standard acoustic sum rules. Lastly, a custom post-processing tool was developed to map momentum-resolved electron-phonon coupling (EPC) directly onto phonon dispersion plots, providing a visual and quantitative representation of EPC strength across the Brillouin zone. These methodological contributions substantially improve the predictive fidelity of superconducting properties under realistic doping and strain conditions. Overall, the methodology demonstrates a state-of-the-art multiscale computational framework, combining electronic, magnetic, and vibrational degrees of freedom to systematically probe and predict the emergent quantum properties of 2D boron-based materials.

2.4. Results of the dissertation and their interpolation

This dissertation presents a detailed and systematic first-principles investigation into the magnetic and superconducting properties of boron-based 2D materials, focusing on β_{12} monolayer and bilayer configurations of β_{12}, χ_3, δ_4, and kagome borophene. The study offers novel insights into how atomic-scale modifications – such as transition-metal adsorption, intercalation, hydrogenation, strain, and charge doping – govern the emergence and tunability of quantum phenomena like magnetism and superconductivity.

In the domain of magnetism, SDFT calculations combined with Monte Carlo simulations reveal that Fe atoms preferentially adsorb at hollow hexagonal (HH) sites of β_{12} borophene supported on Ag(111), forming linear nanostructures that follow the symmetry of the borophene lattice. When Fe atoms are positioned beneath the borophene layer (intercalated between borophene and Ag substrate), the system exhibits enhanced thermodynamic stability. However, due to the significant energy barrier for diffusion through HH sites, surface-adsorbed Fe structures may persist as metastable configurations. Magnetic analysis shows ferromagnetic coupling within Fe chains and antiferromagnetic interactions between chains. The extracted Heisenberg exchange constants were incorporated into classical Monte Carlo simulations, yielding Curie temperatures of 105 K (surface adsorbed) and 30 K (intercalated), indicating that while magnetic ordering is robust, room-temperature magnetism is not yet achieved. The results suggest that substituting Fe with Co – owing to its higher magnetic anisotropy energy – may further enhance T_C.

The microscopic understanding of magnetism in Mn-intercalated bilayer β_{12} borophene was obtained using both the four-state method and TB2J formalism. The later method enabled a detailed analysis of the exchange interactions within an orbitally resolved framework. The first-nearest-neighbor (NN) ferromagnetic coupling is driven by d_{yz}–d_{yz} direct orbital overlap, complemented by $d_{x^2-y^2}$ superexchange interactions mediated via intermediate B-p_z orbitals. Beyond the first NN, superexchange remains the dominant mechanism, particularly along the y-direction, where d_{xy}–d_{xy} and d_{z^2}–d_{z^2} channels contribute significantly. Long-range interactions such as fourth and fifth NNs exhibit complex behavior, including super-superexchange and mixed interaction pathways, indicating the presence of rich magnetic physics and justifying further exploration for spintronic applications.

Regarding superconductivity, the work delivers a critical reassessment of the intrinsic behavior of β_{12} borophene. Contrary to earlier theoretical claims, the thesis establishes that freestanding β_{12} is dynamically unstable and does not support superconductivity under realistic conditions. This behavior stems from the suppression of B-σ state contributions to the density of states (DOS) at the Fermi level, particularly under strain. In contrast, hydrogenated β_{12} borophene (borophane) exhibits dynamical stability and emergent superconductivity. When H atoms adsorb at bridge sites (B–H–B), the structure reaches a superconducting T_C of 6.3 K, which can be enhanced to 28.6 K under +5% uniaxial tensile strain along the hydrogen bridges. This enhancement is directly linked to the increased contributions of B-σ and B-p_z orbitals near the Fermi level. The role of doping was further explored using a realistic field-effect transistor (FET) model, capturing non-uniform doping effects. The study further reveals that standard acoustic sum rules limit stability to low hole doping levels (~0.03 e/B), while more rigorous invariance constraints – such as the Born-Huang conditions – extend dynamical stability up to ~0.12 e/B.

Furthermore, a systematic high-throughput screening was performed on bilayer borophenes intercalated with nine different metal elements across four structural phases. Through DFPT and isotropic Eliashberg theory, 17 stable superconducting configurations were identified, with T_C values ranging up to 27.1 K. Notably, intercalated β_{12} phases, dominated by p_z orbitals, exhibit weak coupling and low T_C (~0.1–1 K), while χ_3, δ_4, and kagome phases – especially those with Ca and Mg intercalation – show significantly higher T_C due to enhanced σ orbital contributions at the Fermi level and strong e-ph coupling. The most promising system, Ca-intercalated kagome bilayer borophene, reaches a T_C of 58 K under anisotropic Migdal–Eliashberg treatment, supported by favorable Fermi surface nesting and strong orbital hybridization. These results underscore the importance of tuning the orbital character at the Fermi level and balancing in-plane and out-of-plane bonding states to optimize superconducting performance.

Finally, a custom post-processing tool was developed to project momentum-resolved electron-phonon coupling strengths onto phonon dispersions, offering an intuitive visualization of mode-selective coupling and enabling identification of dominant phonon channels contributing to superconductivity. This analysis revealed that high-frequency in-plane phonons coupled to σ states play a central role in high-Tc phases.

2.5. Conclusions

This dissertation provides significant advances in understanding and engineering the quantum properties of borophene and its derivatives, positioning these systems at the frontier of 2D materials research. It was demonstrated that β_{12} borophene can host well-ordered 2D magnetic nanostructures like with Fe adatoms forming ferromagnetic chains or Mn-intercalated bilayers exhibiting long-range magnetic order governed by orbital-specific superexchange interactions. These insights mark the first orbital-resolved characterization of magnetism in borophenes and underscore the material's potential for integration into spintronic platforms.

In the realm of superconductivity, the work overturns prior theoretical claims of intrinsic superconductivity in bare β_{12} borophene, offering a critical reinterpretation based on rigorous stability and *e-ph* coupling analyses. Hydrogenated and metal-intercalated configurations emerged as superior alternatives, with borophane showing enhanced critical temperatures under mechanical strain with T_C up to 30 K, and several bilayer phases – most notably Ca-intercalated kagome borophene – achieving robust superconductivity with T_C values exceeding 60 K. These discoveries not only provide a roadmap for experimental realization but also highlight the importance of tuning orbital character, Fermi surface geometry, and chemical stability in designing next-generation 2D superconductors. Collectively, this thesis establishes functionalized borophenes as a promising material platform for future quantum technologies, bridging the fields of spintronics and superconductivity.

3. Final evaluation of the dissertation

3.1. Compilance with the explanation of the topic

The work fully complies with the explanation of the topic.

3.2. Possibility of repeatability

The dissertation is grounded in a robust and transparent computational framework, primarily based on first-principles methods such as SDFT, DFPT, and the anisotropic Migdal–Eliashberg formalism. Standard and widely adopted software packages – Quantum ESPRESSO, VASP, Wannier90, EPW, and Phonopy – form the core of the simulation workflow. All essential computational parameters are meticulously presented and systematically tested throughout the thesis. This level of detail ensures that, in principle, the results are fully reproducible by other researchers.

Nonetheless, certain aspects of the methodology – such as the Wannierization of entangled bands in borophene systems, and the solution of anisotropic superconducting gap equations – are inherently non-trivial and may require expert-level intervention. The accurate construction of maximally localized Wannier functions in these complex systems is particularly sensitive to the choice of initial projections and energy windows, often necessitating manual refinement. Furthermore, select post-processing tasks – such as the momentum-resolved mapping of electron-phonon coupling onto phonon dispersions – were performed using custom-developed scripts, which, while described, are not part of standard distribution packages and would need to be independently replicated.

With access to sufficient supercomputing resources and technical competence in advanced electronic structure methods, the core findings of this work are reproducible. The clarity of documentation, validation of results, and methodological consistency together provide a strong foundation for reliable and repeatable research in this field.

3.3. Future research

The findings of this dissertation open multiple promising directions for future research in 2D boron-based materials. In the magnetic domain, further investigation of transition-metal intercalation in bilayer borophenes – particularly with elements exhibiting large magnetic anisotropy energies – could facilitate the development of robust 2D magnets operating at or near room temperature. Accurate treatment of electron correlation, including the careful choice of the on-site Hubbard **U** parameter, will be essential to capturing the subtle balance between hybridization and magnetic moment retention in these systems. Experimental synthesis and magnetic characterization of such intercalated bilayers remains a crucial next step, where results presented in this dissertation can serve as guidelines.

In the superconductivity domain, the role of **anharmonic lattice effects** – although expected to be moderate in hydrogenated borophene – deserves further theoretical exploration to validate the robustness of predicted T_C enhancements. Experimental efforts are urgently needed to verify the presence or absence of superconductivity in both bare and hydrogen-functionalized borophene phases. Lastly, for metal-intercalated bilayer borophenes, which exhibit high predicted T_C values, particularly in Ca- and Mg-intercalated kagome and χ_3 phases, respectively, experimental synthesis and transport measurements will be vital to confirm theoretical predictions. Future research should also consider device-scale modeling of these systems in realistic conditions, including their interaction with the substrates of choice, and integration into heterostructures and electrostatically

gated junctions, to assess their technological potential in quantum and nanoscale superconducting platforms.

3.4. Dissertation limitations and their impact on the value of the dissertataion

No particular limitations are present.

4. Original scientific contributions
(give clarification: originality (completely new knowledge, addition/expansion of existing knowledge or refutation of existing knowledge), the impact of dissertation results on the progress of the scientific field, the impact results on the profession (directly, indirectly))

This dissertation presents original and impactful contributions across multiple fronts of low-dimensional materials. The magnetic properties of Fe-decorated β_{12} borophene on Ag(111) substrate are explored for the first time beyond schematic treatments, offering a quantitative framework for nanostructured 2D magnetism in substrate-supported systems. In parallel, the work delivers the first microscopic decomposition of magnetic exchange interactions in Mn-intercalated bilayer borophene, introducing a clear orbital-resolved understanding of ferromagnetic coupling in chemically stable configurations. On the superconductivity side, the thesis refutes long-standing theoretical assumptions about intrinsic superconductivity in bare β_{12} borophene. Instead, it identifies hydrogenation as a viable route to both dynamical stabilization and enhanced T_C. Finally, it expands the frontier of boron-based superconductors by identifying a class of intercalated bilayer systems with strong *e-ph* coupling and tunable multigap behavior. The cumulative impact of this work lies in redefining realistic material design strategies for 2D magnetism and superconductivity, with direct implications for spintronic and superconducting device platforms.

5. Opinion and proposal of the jury

The doctoral dissertation of candidate Božidar Šoškić, entitled "Magnetism and superconductivity in two-dimensional (2D) boron crystal structures", presents original and scientifically significant research that contributes both new theoretical insight and critical reassessment of existing knowledge in the field of quantum materials. The results have been published in three peer-reviewed scientific journals:

1. Božidar N. Šoškić, Jonas Bekaert, Cem Sevik, and Milorad V. Milošević, "Enhanced Superconductivity of Hydrogenated β_{12} Borophene", *Nano Letters* **24** (40), 12650–12657, 2024
   American Chemical Society
   DOI: 10.1021/acs.nanolett.4c03845
   URL: https://doi.org/10.1021/acs.nanolett.4c03845
   Q1
2. Božidar N. Šoškić, Jonas Bekaert, Cem Sevik, Željko Šljivančanin, and Milorad V. Milošević, "First-principles exploration of superconductivity in intercalated bilayer borophene phases", *Physical Review Materials* **8** (6), 064803, 2024
   American Physical Society
   DOI: 10.1103/PhysRevMaterials.8.064803
   URL: https://link.aps.org/doi/10.1103/PhysRevMaterials.8.064803
   Q1
3. Božidar N. Šoškić, Srdjan Stavrić, and Željko Šljivančanin, "Ab-initio and Monte Carlo study of Fe-based two-dimensional magnets at borophene supported by Ag (111) surface", *Physical Review Materials* **5** (7), 074001, 2021
   American Physical Society

DOI: 10.1103/PhysRevMaterials.5.074001
URL: https://link.aps.org/doi/10.1103/PhysRevMaterials.5.074001
Q1

with an additional manuscript currently in preparation, further confirming the scholarly value and relevance of the work.

Having carefully reviewed the dissertation, its scientific content, methodological rigor, and published outcomes, the Jury finds that the candidate has met the academic and research standards required for the doctoral degree. The **plagiarism check** has been completed with satisfactory results.

Accordingly, the Jury is pleased to propose to the Council of the Faculty of Natural Sciences and Mathematics, University of Montenegro, to accept the doctoral dissertation of Božidar Šoškić, and to recommend to the Senate of the University of Montenegro the appointment of a Commission for the public defense of the doctoral thesis.

PhD jury for review and evaluation of the doctoral dissertation:

Predrag Miranović

Željko Šljivančanin

Milorad Milošević

Borko Vujičić

Nenad Lazarević

Marin Petrović

Francois Peeters

Date: 07.05.2025