Prof. dr hab. Tadeusz Domański Lublin, 23 August 2023
[Professor, Ph.D., postdoctoral degree holder]
Department of Theoretical Physics
Institute of Physics
Maria Curie-Skłodowska University
20-031 Lublin

Review of the doctoral dissertation of Saeed Samadi Bahnemiri, M.Sc. entitled **"Topological properties of selected IV-VI semiconductor nanostructures"**

The submitted doctoral dissertation is theoretical in nature and concerns the currently important issue of topological states of matter. It includes a detailed analysis of topological insulators in materials based on SnTe and $Pb_{1-x}Sn_xSe$ semiconductors, incorporated into the structures of superlattices, thin films, and quantum wires. The analysis, conducted through a tight-binding approach, includes the examination of symmetry classes, determination of topological invariants, and the definition of band structures and boundary quasiparticles for specific physical systems. The research is carried out under realistic conditions, therefore, the obtained results can be an inspiration for potential empirical verification.

The doctoral dissertation was prepared at the Institute of Physics of the Polish Academy of Sciences in Warsaw under the supervision of prof. dr hab. Ryszard Buczko *[professor, Ph.D., postdoctoral degree holder]*. The dissertation is organized into six comprehensive chapters, wherein the Ph.D. candidate adeptly outlined the objectives and provided helpful introductory information (Chapters 1-3), described the methodology used (Chapter 4), presented the original results of the research (Chapter 5), and provided a succinct summary (Chapter 6). Below I will present an overview of specific fragments of the doctoral dissertation, emphasizing the key accomplishments of the Ph.D. candidate.

In the first chapter, the Ph.D. candidate delved into the fundamental facts and theoretical concepts that go beyond the paradigm of Landau's classification of phase transitions. He referred to the discovery of the quantum Hall effect and Thoulessa's interpretation of this phenomenon, mentioning the close connection of the quantized Hall conductivity, prevalent in strong magnetic fields, and the topological invariant expressed through the Chern number. Then, the Ph.D. candidate cited the idea of the geometric phase, as articulated by M. Berry in the 1980s within the context of band theory. He also touched upon the scenario of Chern insulators realized without a magnetic field, emphasizing the importance of breaking the time-reversal symmetry of crystals. Another fundamental theoretical concept mentioned

in Chapter 1 concerned the implementation of a topological phase without the need to break the time-reversal symmetry on a graphene-type lattice (with an appropriate hop integral to the first and second neighbor nodes), which was proposed by Kane and Mele. The Ph.D. candidate also mentioned the quantum spin Hall insulator in quantum wells based on HgTe/CdTe structures with helical boundary states and two-dimensional and three-dimensional topological insulators, as well as the classification of topology based on symmetries. Following this, the Ph.D. candidate provided a summary of information about the properties of SnTe compounds in which mirror symmetry provides topological protection of the Dirac surface states. By subjecting these materials to structural distortion, magnetic doping, mechanical stress, or precise engineering of nanostructures, it is possible to influence their topological characteristics. This translates into the number and nature of edge quasiparticles, particularly those found in higher-order topological insulators. The primary objective of the current study was to analyze the topological properties of selected nanoscopic structures based on SnTe materials in the presence of selected types of defects. The second chapter delved into the technical aspects of topology (so-called *berology*), and further expanded on the characteristics of various variants of topological insulators.

Chapter three presents information on topological crystal insulators, particularly important in the context of group IV-VI semiconductors. Topological states of matter are distinguished based on the criteria of point group symmetry, e.g. rotational symmetry, mirror symmetry, or their composition. For semiconductors in the SnTe class, the topological nature is primarily determined by reflection symmetry. The Ph.D. candidate elaborated on the theoretical foundation of the topological crystallographic insulator phase predicted in 2012 for the binary compound $Pb_{1-x}Sn_xTe$. Utilizing the $\mathbf{k}\cdot\mathbf{p}$ approach to describe the low-energy spectrum near the four L points of the Brillouin zone, it was anticipated that SnTe and PbTe semiconductors would exhibit Dirac modes. With a change in stoichiometry, a topological phase transition occurs near the critical value x = 0.35. Realistic band structure calculations confirmed the connection to band inversion in the SnTe semiconductor. In three-dimensional crystal structures, the mirror Chern number $C_m = -2$ then implies the emergence of gapless surface states. The Ph.D. candidate highlighted the qualitatively distinct nature of these states on surfaces with Miller indices (111) and (100), illustrated in Figure 3.3. Empirical evidence supporting the presence of such surface states was obtained through photoemission spectroscopy measurements with angular resolution, including spin resolution.

Additionally, the reduction in the number of atomic layers was identified as an influencing factor on the change in topology. This reduction leads to band inversion caused by the hybridization of upper and lower crystal surfaces. The Ph.D. candidate illustrated instances of topological transitions induced by thickness reduction for crystals with surfaces (111) and (100). In the case of the latter, is the realization of the spin Hall effect becomes possible, accompanied by the presence of

helical boundary modes. Thin-layered systems of topological crystal insulators are also notably susceptible to disturbances such as ferroelectric structural distortions, magnetic doping, or mechanical stress. Another specificity of the geometry of *d*-dimensional systems is the possibility of implementing the so-called higher order topological insulators (HOTIs) with a specific number and nature of edge modes, e.g. corner states or hinge states. The Ph.D. candidate presented examples of the potential implementation of HOTIs in group IV-VI semiconductors, such as applying uniaxial stress along the [110] direction in SnTe compounds. Concluding the third chapter, the Ph.D. candidate emphasized the role of symmetry indicators in determining the topological nature, along with a set of suitable topological invariants of individual materials, exemplified by cases like ($Zr(TiH_2)_2$).

The research methodology employed for determining the electronic structure of group IV-VI semiconductors relied on the tight binding model, and Chapter 4 describes the scheme of this method. It references Bloch's theorem and presents the electronic wave function in the Wannier representation (node-centered atomic functions). The Ph.D. candidate outlined the most important matrix elements of the tight bond Hamiltonian essential for describing semiconductors such as PbTe, PbSe, SnTe, and ternary structures like $Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$, considering the basis of *s*, *p,* and *d* orbitals. In particular, the contribution of local spin-orbit coupling was taken into account, whose matrix elements in the *p* orbitals base are shown in equation (4.16). The numerical values of these matrix elements for two-component semiconductors (listed in Tables 4.1 and 4.2) were borrowed from DFT calculations previously carried out in S. Safei's doctoral dissertation under the guidance of the same Supervisor. The spectra of various geometric structures were determined iteratively within the Green's function formalism. The main object of interest of the analysis performed was the spectral function [defined by equation (4.21)] and topological properties. On the other hand, the spectrum of $Pb_{1-x}Sn_xTe$ and $Pb_{1-x}Sn_xSe$ semiconductors was determined using the virtual crystal approximation, self-consistently incorporating contributions from components with x and $1 - x$ concentrations. During the final defense of the dissertation, I would like to ask the Ph.D. candidate to present the algorithm of the above-mentioned approach, taking into account the reliability of the determined dispersion relations, since the approximation is local.

The set of original findings achieved by the Ph.D. candidate is described in Chapter 5. In this section, the characteristics of the energy spectrum (in terms of topological properties) of selected geometric structures based on SnTe and $Pb_{1-x}Sn_xSe$ semiconductors were examined. In particular, the following were considered: a) superlattices formed by a pair of defective planes, b) layered systems with a single plane defect, c) quasi-two-dimensional Hall-type structures, and d) nanowires with a pentagonal and square cross-section. The results for the first two cases were published in the article by S. Samadi, R. Rechniński, R. Buczko, Phys. Rev. B 107, 205401 (2023).

Section 5.1 explores the energy structure and topology of a three-dimensional crystal. This crystal's unit cell incorporates two layer defects (commonly knowns as twin planes), which result from the rotation of the planes relative to the selected direction by an angle π (180^o). Figure 5.1b illustrates a crystal with such layered defects formed along the [111] direction. The Ph.D. candidate highlighted that these superlattices are characterized by: reflection symmetry with respect to (111), mirror symmetry {110}, and rotational symmetry C_3. Additionally, in unit cell configurations with identical ionicity, there exists inversion symmetry, whereas in configuration with mixed ionicity, such symmetry is absent. Figure (5.2) illustrates the hexagonal shape of the three-dimensional Brillouin zone. The electronic structures for each ionicity type, determined along the directions of high symmetry for a cell composed of two hundred layers (with half separated by layer defects), are depicted in Figures (5.3)-(5.5). Table (5.1) provides the topological characteristics, presenting the values of the Z_2 indices and the mirror Chern numbers C_m obtained through the Fu-Kane procedure (for superlattices with identical ionicity) and the Fukui method (for mixed ionic configurations). For more detailed insight into the origin of topological invariants, the Berry curvature was examined on cross-sections of the Brillouin zone in ΓMK and ALH planes. Extreme values of Berry curvature were found to occur near points of high symmetry. By summarizing the Berry flux from the vicinity of three M points and Γ point, the mirror Chern numbers from Table (5.1) were recreated. The value of the topological invariants determines the number of boundary states and for the current case, the existence of these surface states for a semi-infinite crystal was confirmed by calculations of the spectral function along the $(1\bar{1}0)$ and $(11\bar{2})$ surfaces. For various ionic configurations, the presence of Dirac cones within the semiconductor gap was found, and the number of these cones aligned with the value of topological invariants. The spectral functions for $(1\bar{1}0)$ and $(11\bar{2})$ surfaces are shown in Figures (5.9) and (5.10), respectively.

In the next Section 5.2, the influence of a single layered defect on the topology of energy states in a finite-thickness crystal is examined. The calculations were specifically performed for a system comprising 121 layers, equating to a thickness of 21.8 nm. The layered defect was positioned in the central part of the system with Miller indices (111), and its distance from the lower/upper surface was large enough to render the hybridization effects negligible. Based on the calculations performed, the band structure was determined for both cationic and anionic configurations of the system, assuming identical ionicity for the surface and defect layers. Figure (5.12) shows the energy spectrum for each configuration, highlighting the dispersion lines originating from the surface layers, the defect layer, and the rest of the system. The surface states of both ionic configurations indicated the presence of four Dirac cones: one around the Γ point and three around the M_i points of the Brillouin zone. The boundary spectral functions along the $[11\bar{2}]$ direction of the Brillouin zone are shown in Figure

(5.13), illustrating the spectral weight of the ±*i* subspace. To assess the topology of the layered defect, a disruption in the surface states was induced by applying a disturbance potential. The results obtained in the presence of a non-magnetic potential (applied with the opposite value for the lower and upper layers) are shown in Figure (5.14). Subsequently, the mirror Berry curvature of the anionic and cationic layer defects was investigated by inducing a break in the Dirac mode with a magnetic field (via 0.5 eV Zeeman splitting). The calculations revealed fractional values of the Berry flux around the high symmetry points $\bar{\Gamma}$ and $\bar{M}$. As a result, the mirror Chern numbers were determined as $C_m = 2$ for the cationic configuration, and $C_m = 1$ for the anionic configuration, respectively. A helpful procedure for analyzing the topology of the band structure (considering the contribution of defect states, surface states, and the rest of the studied systems) was developed by Mr. Rafal Rechciński, co-author of the publication in Phys. Rev. B 107, 205401 (2023). The method for determining the projected Berry curvature is outlined in Section 5.2.3 of the doctoral dissertation, with the detailed calculation scheme presented in Appendix C of the mentioned publication.

Section 5.3 analyzes the conditions for the feasibility of the quantum spin Hall (QSH) effect in thin systems based on SnTe semiconductor layers. For this purpose, quasi-two-dimensional structures composed of several to several dozen layers were considered, in which the hybridization of the edge surfaces leads to the inversion of the bands around the Γ point, which is responsible for the QSH phenomenon. The physical basis for this size effect-based mechanism was previously formulated by the Supervisor and colleagues [New J. Phys. 17, 063041 (2015)] for regular crystal structures of the SnTe semiconductor. The Ph.D. candidate generalized this scenario to the case of systems with a centrally built-in layer defect, for which, in addition to the topological invariant Z_2, the mirror Chern number C_m can be additionally determined. Based on the calculations performed for the *spd* orbital model, the oscillatory behavior of the energy gap around the Γ point (and the monotonic reduction of the energy gap around the *M* point) was examined as a function of the number of crystal layers, indicating the areas of the topologically non-trivial phase $|C_m| \neq 0$. The results obtained for various configurations of the boundary surfaces and the layered defect are presented in Figure (5.19). Berry curvature analysis was performed to illustrate the effect of the system thickness (i.e., the number of crystal layers) on C_m. Figures (5.21) and (5.22) show the results for individual ionic configurations, indicating that the hybridization of the boundary layers plays a fundamental role in the transition to the topological phase and the implementation of the QSH phenomenon. Additionally, the Ph.D. candidate determined the spectral function of boundary states, confirming the presence of helical modes around the $\bar{\bar{\Gamma}}$ point in systems with the number of layers corresponding to the non-zero C_m invariant.

Section 5.4 delves into the topological characteristics of SnTe and $Pb_{1-x}Sn_xSe$ semiconductor nanowires featuring pentagonal and square cross-sections. By examining the band structure of SnTe quantum wires with a pentagonal cross-section, it was shown that above

a thickness of 14 nm, Dirac-type modes occur around a $\bar{\Gamma}$ point propagating along the core and edges. Edge modes manifest exclusively in systems with cationic ionicity of segments connecting trigonal components of nanowire, and they are closely linked to the occurrence of the topological crystal insulator phase. There are also surface states in the band structure that couple to edge modes (even as the nanowire thickness increases). Among the five edge states, only one pair exhibits the Dirac type, as demonstrated in Figure (5.30) through C_5 symmetry analysis. Conversely, for nanowires with anionic ionicity, the absence of band inversion indicates the presence of a non-topological phase. Analogous properties were found in the $Pb_{1-x}Sn_xSe$ semiconductor, where the core Dirac mode develops around a point in cationic configurations of quantum wires with a thickness above 28.6 nm. It has also been shown that the incorporation of $(21\bar{1})$ domain walls on each of the five trigonal components of the nanowire does not qualitatively change the topological properties of the system, as long as the C_5 symmetry is maintained. The Ph.D. candidate presented an argument based on the low-energy model of edge states, explaining why only one pair of such modes exhibits Dirac characteristics. The final segment of Chapter 5 addresses the band structure of quantum wires of the SnTe semiconductor with a square cross-section. In this scenario, geometries with rotational symmetry C_4 and the variant of symmetry 4_2 depicted in Figure (5.38b) were considered. In both cases, the calculations showed effective hybridization of surface states, preventing the occurrence of massless modes. Consequently, the Ph.D. candidate concluded that only in nanowires with cross-sections characterized by C_n rotational symmetry with an odd number n can a non-degenerate pair of Dirac-type edge modes exist. In other cases (such as those with even numbers of n), hybridization effects induce a break in the dispersion of edge modes.

In the summary (Chapter 6), the Ph.D. candidate compiled the most important findings from theoretical calculations carried out on three-dimensional superlattices, quasi-two-dimensional Hall systems, and quantum nanowires. He emphasized the key role of the symmetry of individual systems, which determines the emergence of topologically protected edge modes at the transition induced by band inversion. The adequate topological invariant in superlattices with a double and single plane defect is the mirror Cherna number, the value of which is determined by the cationic or anionic configuration of the plane defect and then translates into the topological characteristics of the band structure. The Ph.D. candidate demonstrated that the topological impact of a plane defect is also manifested by the spin quantum Hall effect with helical edge modes. This effect is predominantly realized depending on the thickness of thin systems. Moreover, the Ph.D. candidate identified the conditions for the topological crystal insulator phase in semiconductor quantum nanowires with various cross-sections, which is realized for odd rotational symmetry C_n. The candidate exemplified this effect on the example of quantum wires

with a pentagonal cross-section (where the topological phase takes place only in the case of cationic ionicity of the segments connecting the trigonal components of the nanowires) and a square cross-section (where the topological phase cannot be achieved).

The editorial quality of the doctoral dissertation does not pose significant concerns. However, as a reviewer, I will highlight some of the errors I observed: [page 35] *Typically, The TCIS! Typically, the TCIS;* [page 36] *are classified as a narrow → are classified as narrow; [page 36] They have been long attracted attention due to its unique → They have attracted attention due to their unique;* [page 37] *First principle calculations (see Fig. 3.1) shows → First principle calculations (see Fig. 3.1) show;* [page 62] *induce a new topological phases → induce new topological phases;* [page 71] *mirrir → mirror;* [page 75] *However, This → However, this;* [page 80] *investigating of topology → investigation of topology;* [page 87] *helps explain → helps to explain;* [page 104] *is depended on → is dependent on.* The above comments do not have the slightest impact on the understanding of the content of the doctoral dissertation and do not change my very positive assessment of the entire work.

The submitted doctoral dissertation makes a significant contribution to understanding the topological nature of the band structure of semiconductor nanosystems based on elements from groups IV and VI of the periodic table. The Ph.D. candidate conducted a meticulous symmetry analysis, identified topological invariants using appropriate model criteria, and thoroughly examined the band structure and characteristics of boundary states. The doctoral dissertation has been carefully prepared in English and meets the customary and legal requirements specified in the Act on Higher Education and Science (Journal of Laws of 2020, item 85, as amended) for the conferment of a doctoral degree in the field of *physical sciences*. Based on these considerations, I hereby request the Scientific Council of the Institute of Physics of the Polish Academy of Sciences in Warsaw to admit Saeed Samadi Bahnemiri, M.Sc., to the public defense and subsequent stages of his doctoral dissertation.

Signed by / Podpisano przez:

Tadeusz Krzysztof Domański
Maria Curie-Skłodowska University in Lublin

Date / Data: 2023-08-23 16:51