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

The doctoral dissertation of Saeed Samadi Bahnemiri, M.Sc., has been prepared in English and spans 120 pages. It incorporates 151 literature references and features 62 illustrations. The formal structure of the work includes an introduction, three chapters introducing the theoretical methods used (Chapter 2, Chapter 3, and Chapter 4), followed by an extensive Chapter 5 containing the research results obtained by the Ph.D. candidate. The formal division of the work is uneven, with Chapter 5 covering over half of the dissertation, while Chapter 4 is only 8 pages long. From the reader's point of view, it would be easier to engage with a manuscript of a more balanced structure. Nevertheless, the layout remains logical and effectively reflects the main theses of the dissertation.

Assessment of the introductory section of the work.

The introductory part of the work, consistent with the adopted title of the entire dissertation, naturally covers a rather broad subject matter. It discusses the topological properties of materials in band description (Chapter 2), specific properties of crystals and nanostructures made of type IV-VI semiconductor materials (Chapter 3), along with methodologies for modeling electronic states in crystal structures (Chapter 4). While the choice of these subjects is entirely appropriate, the presentation does have a number of shortcomings.

Chapter 1, titled "Introduction", briefly presents the most important parts of the dissertation. In some statements, the author oversimplifies the explanation to the point where it becomes difficult to comprehend. The sentence "topological classification (...) focuses on the examination of global characteristics employing topological invariants", seems to contain a logical error of explaining an unfamiliar (to the reader) concept of "topological classification" using the same concept but from a different perspective, namely "topological invariants". As a result of the author's similar tendency to condense statements excessively, the sentence "the role of time-reversal symmetry breaking in maintaining the crystal's periodicity" becomes inaccurate. Time-reversal symmetry definitely cannot be the cause of maintaining the crystal structure's periodicity. On a positive note regarding the content presented in the "Introduction", I would highlight the clear presentation of the purpose of the work and the synthetic approach to the obtained results.

Chapter Two's title, "Topological states of matter", is somewhat overstated by the author. The content presented actually concerns a much more limited scope, specifically topological phases related to the band description of non-interacting electrons. Typically, discussions about "topological states of matter" encompass a broader range, also in the context of interacting systems, such as states in the fractional quantum Hall effect.

The presentation of the theoretical content in this chapter resembles a summary of conventional textbook approaches. The author primarily relies on well-established derivations without significant innovations, and ignores more intricate results (e.g., failing to provide justification for the equivalence of the Berry curvature forms in (2.12) and (2.16)). A strength of this chapter is the author's creation of illustrative drawings and charts. These visuals are very nicely designed, clear, and thoughtfully selected. An interesting and innovative element is the result presented in subsection 2.6.3.5. Using a simple Hamiltonian model, the author tests a numerical method (presumably developed specifically for this work) that allows to determine topological invariants for a band structure lacking inversion symmetry. This departure from conventional textbook content is supported by an illustration, Fig. 2.10, containing a color map depicting the spin-resolved spectral function of a topologically trivial ($\upsilon=0$) and non-trivial ($\upsilon=1$) system.

The Fukui-Hatsugai method provides the author with a numerical study of topological invariants, as well as insight into the momentum dependence of Berry's curvature. It is the author's central methodological tool, and as such, in my opinion, should be carefully presented. The numerical implementation of the general formulas from the introduction (e.g. those mentioned here (2.12) or

(2.16)) is not immediately apparent and encounters certain obstacles. The author treated the description of the difficulties and the solution used very briefly (a single paragraph on page 29), as a result of which this section of the work is practically illegible. As part of the defense, I would expect the author to expound on this method in sufficient detail to confirm his theoretical expertise.

The next chapter (Chapter 3) bears the title “Topological crystalline insulators”, aptly reflecting its content. It reviews results from the literature over the last decade on topological insulators with states protected by crystal (TCI) symmetries. In this instance, the illustrations accompanying the text, although meticulously prepared, are sourced from the works of other authors (including the supervisor, Professor Buczek) and are cited as scientific quotations. The review, while necessarily brief, is well-executed, and the examples chosen align with the needs of the entire dissertation. It is certainly valuable to cover issues that have recently been actively discussed by numerous authors, regarding hinge states and higher-order topological insulators. However, I feel that this chapter is missing the presentation of material demanding the author's unique contribution. Certainly, some of the illustrations used for the introductions included in this chapter could have been prepared (and tested against the literature) using the methods developed for the research purposes in Chapter 5.

A notable weakness in this chapter lies in the absence of an introduction that familiarize the reader with the issues of specific types of systems, which became the main axis of the research reported in Chapter 5 of the dissertation. Concepts like twin plane defects (TP for “twin planes”) and superlattices constructed from such defects (TSL for “twin superlattices”) do not appear until Chapter 5. When they are introduced, it is done in an expert manner, condensed and providing limited explanation to the reader. The appropriate place to announce, define, and illustrate exemplary TP or TSL would be in this introductory chapter, it would also serve to better justify the undertaken research.

The shortest section of the work (Chapter 4) is titled “Methodology”. It mainly provides an introduction to the modeling of electronic states in IV-VI semiconductor structures – through the tight bond approximation, general Slater-Koster parameterization, and summary tables of parameters relevant to the models used in the study. I have no comments in regard to this part of the chapter.

Moving forward, the author briefly revisits the method for calculating the Green's function and the single-particle density of states in the geometry of a semi-infinite system. Although the author had to use this method for specific calculations later in the work, the report presented to the reader is rudimentary. The author writes generally “this equation can be used to derive numerous other equations that combine block matrices” yet fails to elaborate on the derived equations, the derivation process, or the numerical solution methods. Of course, a link to the original work is included, but the reader (reviewer) does not receive confirmation of the author's theoretical proficiency in the methodology used. Moreover, a fellow Ph.D. candidate seeking to learn something about calculating surface densities of states would not benefit much from this section.

Summary of comments about the introductory section.

The author exhibits a fundamental understanding of theoretical issues at the basic level required of a Ph.D. candidate, but does not demonstrate proficiency or a desire for in-depth understanding of the issues presented.

Assessment of the research section of the work.

Chapter 5 encompasses the research segment of the study. The author presents theoretical results derived for nanostructures composed of II-VI semiconductors. The primary focus of the research revolves around structures with single or multiple twin plane defects. This chapter contains meticulously prepared illustrations, charts, and a lot of various results, all of which are reported in detail.

Section 5.1 is a segment built upon extensive collaborative efforts published with the supervisor. The method of presentation and the substantive content of the demonstrated results do not raise any major concerns. The study in this section delves into states within twin plane superlattices, specifically: the volumetric band structure of the systems, the topological properties of this structure in terms of Chern mirror invariants, and the boundary states of the superlattices. The visual aids, including figures and charts illustrating the obtained results, are provided as a scientific citation from the published work. These illustrations are very carefully thought out. They suggest that the Ph.D. candidate, when preparing the publication and dissertation, has not only achieved proficiency in generating results but also has displayed expertise in effectively illustrating and selecting them to produce a high-quality scientific manuscript.

Section 5.2 applies a very similar scientific method, but to a single TP confined in plate geometry. This analysis allows us to better illustrate the role of TP in the formation of topological states, and is complementary to the results from Sec. 5.1. It was included in the dissertation for completeness of presentation, but at the same time it effectively documents the author's own contribution to the research. The results from Chapter 5.2 seem to confirm previous theses, and they do not bring any qualitatively new effects.

A more ambitious cognitive attempt is presented in the content of Chapter 5.3. The author seeks to identify the optimal configuration with TP present in a thin plate, so that it is possible to achieve QSHE (quantum spin Hall effect) at the edge states. The results are interesting, obtained for more realistic models of tight binding, and may become a guide for experimental groups. I do not see a clear conclusion that the presence of TP qualitatively improves the conditions for observing QSHE. The topic probably requires a broader exploration of model parameters and extension of research to obtain publication-quality results. However, this subchapter has its place in the text of the dissertation, containing an original extension of the Ph.D. supervisor's previous results. Paradoxically, the observation of flat edge bands (Fig. 5.23 f) may be the most interesting result of this line of research. For the purposes of public defense, it is worth considering whether, and to what extent, flat edge bands are a stable function of the parameters and a distinct (or unique) feature of the tested systems.

The last chapter of the work (Chapter 5.4) contains a detailed analysis of electronic states in nanowires composed of SnTe class materials. The objective is to search for suitable nanowire geometries and parameters for observing exotic hinge states and core states. This topic is actively debated within the research community, and the author's results from this chapter are certainly extensive and exhaustive enough to become the material of a separate publication in a prestigious international journal. The nanowires under consideration exhibit a distinctive five-fold symmetry. This atomic configuration is possible to construct by using TP defects five times, the resulting structure has almost no stress. The proposed structure therefore elegantly connects with previous research on the properties of topological states in the presence of TP defects. I commend the substantive richness of this chapter and the innovative discussion on topological states in the presence of non-obvious 5-fold symmetry.

Summary of the assessment of the research section.

The Ph.D. candidate has achieved scientifically important results and was able to present them in a thoroughly accurate scientific text within this dissertation. He correctly applied and consistently developed the adopted methodology. The described results document progress in the theoretical understanding of advanced issues in the physics of topological states protected by various crystal symmetries.

Conclusion.

I certify that the work submitted for evaluation, prepared by Saeed Samadi Bahnemiri, M.Sc., with the title “ “ meets the statutory requirements for doctoral dissertations. I am confident that the scientific quality attained by the candidate aligns with the customary expectations outlined in the doctoral procedure. I request that the proceedings be progressed to further stages, including a public defense of the dissertation.

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