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Institute of Theoretical Physics

Wrocław, 21 April 2023

Review of the doctoral dissertation of **Mr. Rajibul Islam, M.Sc.** entitled
Topological phases of 3D superlattices and 2D materials: theoretical modeling

The doctoral dissertation of Mr. Rajibul Islam, M.Sc., consists of three multi-authored articles published in peer-reviewed scientific journals. In all these publications, the Ph.D. candidate is the first author. All the papers are computational and are devoted to the study by "first-principles" methods of various 2- and 3-dimensional materials from the point of view of the topological phases present in them.

The statement of own contribution, presented by Mr. Islam, together with the consistent statements of the co-authors, make it possible to clearly distinguish the individual contribution of the Ph.D. candidate to the published works, and even indicate his sole contribution to the implementation of research tasks and significant participation in the formulation of research goals, interpretation of results and editing texts. I state, however, that the presented statements of the Ph.D. candidate and co-authors about the nearly exclusive contribution of Mr. R. Islam to the creation of the publication are in contradiction to the explicitly stated equal contributions of the first two authors in the second of the presented publications. This proves that the Ph.D. candidate committed nothing less than scientific dishonesty in one of these declarations of contribution. Given this serious doubt, I believe that the publication in Phys. Rev. B **104**, L201112 (2021) should not be considered as the basis for a degree (although I discuss it below as well as the other two). Nevertheless, the doctoral dissertation limited to the other two publications still meets the formal requirements of Art. 187 Sec. 3 of the Act on the *Law on Higher Education and Scienc*e, if understood as a separate part of the collective work, which are the other two published articles, in the case of which there are no formal grounds to question the Ph.D. candidate's contribution.

The articles presented as the basis for conferring a degree were – following a commendable custom – preceded by a general introduction, in which the Ph.D. candidate first introduces the topic of topological phases of matter (Chapter 1), and then outlines the basics and methodology of DFT calculations used in his scientific work (Chapter 2). This introduction, and especially its first part, is weak and even sloppy in terms of language, editorial, and content. It contains undefined symbols (e.g. Theta under formula (1.4)), imprecise expressions (e.g. *the Hamiltonian can be split into two sub-spaces* or *mirror operator is invariant on a fixed plane*), errors in formulas (e.g. index *k* instead of *R* in equation (2.30)), as well as completely vague statements, such as *The band inversion can be tuned with impurity of strain, it also influences the size of the nodal line which is a interesting platform to study correlated materials and flat band physics*. I do not understand how the Hamiltonian formalism of equation (2.33) can be more accurate than (2.32) since they only differ in a trivial change of basis.

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Wybrzeże Wyspiańskiego 27
50-370 Wrocław

T: +48 71 320 25 79

wppt.ift@pwr.edu.pl
www.ift.pwr.edu.pl
www.pwr.edu.pl

REGON *[statistical No.]*: 000001614
NIP *[taxpayer ID No.]*: 896-000-5851
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The Ph.D. candidate does not use punctuation after mathematical formulas, does not monitor the indentation of the text after formulas, and does not care about the spacing between the reference and the preceding text. From the substantive point of view, the presentation not only does not contribute anything new in terms of the available review papers, but even in many places it is incomprehensible without reference to such works. This hermeticity of the text is particularly annoying for someone who – like me – has only general knowledge in the area of the research presented by the Ph.D. candidate. In particular, I missed the newer aspects of the current state of knowledge and the explanation of technical terms, both very simple, such as the structure of the 1H, 1T' phases, and more complex, such as *3D flat bands*. From an article by Lau *et al.*, Phys. Rev. X 11, 031017 (2021) I managed to understand roughly how such bands appear in topological semimetals with nodal line semimetals in the presence of stress, but this information cannot be obtained from the introduction to the dissertation, although this issue is presented as the main motivation of the work. It seems to me that the aforementioned article is crucial for understanding the purpose and meaning of a large part of the Ph.D. candidate's work and should even be referred to by him in the introductory part of the dissertation. The most surprising editorial clumsiness is the heading of Chapter 1.2, followed by no text. It is a pity because here the Ph.D. candidate could formulate the general aim of the work, synthetically present his achievements and emphasize the thematic coherence of the presented articles (fortunately, in this case, there is no doubt of this). As it seems, the introduction is not part of the dissertation and formally it is probably not subject to evaluation, but it is difficult not to comment that the inability to edit a short introductory text is not a good indicator of the "ability to conduct scientific work independently" by the Ph.D. candidate, required by law and customarily expected. Moreover, the obvious inconsistencies in the formulas raise concern as to his understanding of the foundations of formalism, i.e. "general theoretical knowledge" (quotes from the Act). The discussion of the doctoral dissertation conducted as part of the public defense should dispel these doubts.

I will now discuss the three scientific articles constituting an essential part of the dissertation. Given the statement of the Ph.D. candidate and co-authors, I assume that at least in the case of the first and third papers, all of the presented results, as well as the formulation of the problem, interpretation of the results, and editing of the text, should be attributed to the Ph.D. candidate.

In the first of these papers [R. Islam et al., Phys Rev. Res. **4**, 023114 (2022)], the author performs a computational characterization of the topological phases in short-period HgTe/CdTe and HgTe/HgSe superlattices, also in the presence of stresses (epitaxial and externally generated). The calculation method used is DFT (Density Functional Methods) and tight binding models derived from them – as I understand it, the latter are used for practical and computational reasons. The main motivation of the research is the search for topological semimetallic phases with nodal line semimetals

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(NLS), in which non-dispersive bands on the Fermi surface can occur, which in turn opens up a huge space for the appearance of various interesting phases in correlated systems of many particles. The present paper addresses this interesting topic initiated by an earlier article [Lau et al., Phys. Rev. X 11, 031017 (2021)] and, although conceptually it does not seem to contribute anything new to the development of the theory as such, it offers a very systematic and complete characterization of topological phases in the studied systems. The basis of this analysis is the study of the band structure, although Berry streams are also illustrated, which show a topological structure. Among the identified phases, there are sought NLS phases, but also – in the case of HgTe/HgSe – many other known topological phases, between which the system passes under the influence of deformations. I cannot assess to what extent the assumed deformations (at the level of 15% change in the lattice constant) are realistic, but regardless of this, such material characteristics seem important and interesting to me. I consider the scope of computational characterization presented in this paper to be impressive. The article also includes a good complete discussion of the discussed structures in terms of their symmetry, followed by a systematic analysis of band structures and a physical discussion of their origin, which indicates a good orientation of the Ph.D. candidate in this area of solid state physics.

Reading this article in light of the outline of the methodology presented in Chapter 2 of the introduction to the dissertation raises, in my opinion, one formal doubt. The Psi functions, rightly called Kohn-Sham orbitals by the author (above equation (2.13)) are in a sense an artificial creation corresponding – ambiguously – to electron density, which is the only quantity determined directly in DFT calculations. I noticed with concern that in the further argument (I mean Chapter 2 of the introduction to the dissertation) these functions are treated as real wave functions (Bloch), and finally above equation (2.24) they are called *actual wave function* and used to characterize the topological features of the structure band. I'm not in the slightest an expert on DFT calculations, but it doesn't seem right to me, at least without further justification. As far as I know, there are methods for reproducing the actual Bloch functions from the DFT results obtained under the PAW method, but they are not trivial. On the other hand, in the discussed article, at the end of Chapter IV, there is a sudden and devoid of any methodological commentary jump from band structures to topological properties of wave functions, and the methodology in this respect, given in one sentence in the last paragraph of Appendix A, is defined only by reference to the functionality of specific computational packages which seems scientifically incorrect to me.

In the next paper [R. Islam et al., Phys Rev. B **104**, L201112 (2021)], the Ph.D. candidate studies the electronic structure of single- and multi-layer materials made of MSi_4Z_4 compounds, where M is molybdenum or tungsten, and Z is nitrogen or arsenic, using DFT computational methods. This is an interesting class of materials, also because they are produced by epitaxy

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rather than exfoliation (there are no bulk parent crystals). In this work, the Ph.D. candidate also demonstrates the thermodynamic stability of such structures as well as the corresponding bulk materials. These are materials with a hexagonal structure, in which there is no inverse symmetry in the case of one layer, while such symmetry appears in a two-layer system, and disappears again when an electric field is applied along the growth axis. This results in the valley-spin structure, well-known from analogous systems, and in addition, it was shown in the work that, depending on the chemical composition, the investigated single-layer structures may have straight- or skew-gap characteristics. The work seems to present rather routine calculations, and its importance is, in my opinion, mainly due to the fact that it deals with new and interesting material. I have two technical questions. First of all, the introduction to the publication given by the Ph.D. candidate (very neat this time) shows that layered materials of this type appear as a result of the passivation of molybdenum nitride with silicon, and therefore always on a MoN substrate. However, the calculations seem to be made on detached structures. Wouldn't the substrate have a decisive influence on their properties? Certainly, the presence of the ground breaks the symmetry of the inversion. Second, the jump to 99.9% almost exactly at the Gamma point in Fig. 2e is strange. Isn't that a numerical artifact?

In the last of the papers included in the dissertation [R. Islam et al., Phys Rev. B **106**, 245149 (2022)] Mr. Rajibul Islam proposes and studies (again by DFT methods) a two-dimensional material with the same stoichiometry as before, but with a different spatial structure. It computationally proves its relative stability by analyzing both phonon dispersion relationships and *ab initio* molecular dynamics results. It shows that spin-orbital interactions lead to the opening of a gap at the band-crossing points, leading to the structure of the quantum spin Hall insulator. It also shows that the gap is closed in this material and a topological phase transition occurs depending on the external electric field. The results presented here are interesting and original. Proposing a new material based on computational results seems to me a significant scientific achievement. I am curious to what extent (statistically speaking) such computational predictions are later confirmed experimentally. As for the detailed results, I am not convinced to what extent the study of the stability of the detached layer is reliable. I suspect that in the case of the existence of two phases with similar stability, the structure of such an epitaxially formed material is determined primarily by the substrate, and the Ph.D. candidate does not study this, focusing – as I understood – on the detached layer.

If the scientific problem being the subject of the dissertation is to consider the computational examination of the properties of selected 2- and 3-dimensional materials showing topological phases, then undoubtedly it should be considered that this problem was originally solved by the Ph.D. candidate in the sense that the characteristics given by him were not known before. The undoubtedly original element is the proposal of a new two-dimensional material showing controlled topological properties. The presented analyses

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are extensive, complete, and prove a good knowledge not only of the computational craft of DFT but also of the relevant areas of solid-state physics. The presented dissertation is overshadowed by the glaring inconsistency in declaring the participation of co-authors, which is deeply objectionable to me, but I do not intend to hold the novice scientist fully responsible for this fact. Even without this one dubious article, the dissertation would meet the requirements for doctoral theses.

In view of the above, my rating of the doctoral dissertation of Mr. Rajibul Islam, M.Sc., is positive.

[illegible signature]
Professor Paweł Machnikowski

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