

MERIT / MERIT-WINGS Internship report (FY2025)

Graduate School of Science, Department of Physics, PhD Program (2nd Year)

MERIT-WINGS Program, 11th Cohort

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【Overview】

- **Period: September 13, 2025 – March 13, 2026**
- **Host Institution: nextnano GmbH (Munich, Germany)**
- **Research Topic: Simulation of Topological Insulators using nextnano**

【Research Background】

In recent years, topological insulators have attracted significant attention as a class of materials exhibiting novel electronic states originating from the topology of their band structures. These materials are characterized by an insulating bulk and dissipationless conducting states at surfaces or interfaces, making them promising candidates for applications in spintronics and quantum information devices. In particular, narrow-gap semiconductors such as HgCdTe and HgTe have been extensively studied, where band inversion can be induced through compositional tuning and quantum well engineering, leading to a phase transition from a conventional insulator to a topological insulator. The emergence of such topological phases is highly sensitive to slight variations in material composition and structural parameters, necessitating precise and quantitative analysis for their design and understanding.

More recently, topological phases have also been reported in heterostructures involving InAs-based materials, further expanding the range of candidate systems. In particular, a study published in 2025 demonstrated the relationship between band structure and topological properties in InAs-based systems, suggesting that similar physical mechanisms can be realized across different material platforms.

However, experimental investigation of topological insulators requires sophisticated sample fabrication and low-temperature measurement techniques, making exhaustive exploration of parameter space challenging. Therefore, theoretical modeling and numerical simulation play a crucial role in guiding experimental design. In particular, band structure calculations based on the $k \cdot p$ method and envelope function approximation have been widely used to analyze band inversion and the emergence of edge states in quantum well structures. Moreover, implementing these theoretical models within numerical simulation tools enables quantitative analysis of complex material systems and device structures.

Nevertheless, such simulations are highly sensitive to material parameters and model assumptions. Variations in literature values and interpolation schemes can significantly affect the results, and improper interpretation without considering model validity may lead to incorrect physical conclusions. Therefore, to advance the design and understanding of topological insulators, it is essential to treat material parameters, theoretical models, and simulation results in a consistent and physically rigorous manner.

In this study, numerical simulations of semiconductor nanostructures using nextnano were conducted to analyze band structure evolution and the conditions for the

emergence of topological phases, with the aim of clarifying the relationship between theoretical models and computational results.

【Research Methods】

In this study, numerical simulations of semiconductor nanostructures were performed to quantitatively evaluate the conditions for the emergence of topological phases and the evolution of band structures. The primary focus was on HgCdTe-based quantum well structures and related low-dimensional systems, where the effects of compositional and structural variations on electronic states were systematically investigated.

First, material parameters used in the simulations were carefully examined and refined. Since parameters such as band gap, effective mass, and spin–orbit coupling directly influence the results, multiple literature sources were compared to assess their consistency and applicability. For alloy systems, particular attention was paid to interpolation schemes and their underlying physical assumptions, as they critically affect the band inversion conditions.

Next, band structure calculations based on the $k \cdot p$ method were carried out to analyze electronic states in quantum well structures. Energy dispersion relations, density of states, and spatial distributions of wave functions were evaluated. The presence of band inversion was determined by examining the ordering of conduction and valence bands. By systematically varying parameters such as composition and well width, the transition from a conventional semiconductor phase to a topological phase was investigated.

Furthermore, simulation results were interpreted in comparison with theoretical models and prior studies to verify their validity. Rather than relying solely on numerical outputs, emphasis was placed on understanding the assumptions and limitations of the models to derive physically meaningful conclusions.

In addition, particular attention was given to reproducibility and reliability. Simulation inputs, structural parameters, and computational settings were carefully documented, and consistency was confirmed through repeated calculations. Sensitivity analysis was also performed to evaluate the impact of small parameter variations on the results.

【Research Results】

Through this study, the evolution of band structures in HgCdTe quantum well systems was quantitatively analyzed, and the conditions for band inversion were successfully reproduced numerically. Furthermore, by applying the same framework to the InAs-based system reported in a 2025 study, the band structures and topological properties described in the literature were successfully reproduced. These results demonstrate that, with appropriate parameter selection and modeling, the emergence of topological phases can be consistently described across different material systems.

The analysis also revealed that the emergence of topological phases is highly sensitive to material parameters and structural conditions. In particular, slight variations in alloy composition and well width significantly affect band ordering, ultimately determining whether a topological phase appears. This finding highlights the necessity of precise parameter control in device design.

Moreover, this work provided a deeper methodological understanding of numerical simulations. It was recognized that simulation results strongly depend on input parameters and model assumptions, and therefore require rigorous validation through literature comparison, careful documentation, and reproducibility checks. In addition, the importance of critically interpreting simulation results in the context of theoretical models was emphasized.

Overall, this study establishes a quantitative framework for analyzing band inversion and topological phase transitions using numerical simulations, and provides a foundation for integrating experimental, theoretical, and computational approaches in the study of topological materials.

【Reflection】

Through this study, a quantitative understanding of band structure evolution and topological phase transitions in topological insulators was achieved using numerical simulations. In particular, reproducing band inversion in HgCdTe and InAs-based systems provided concrete insight into the strong dependence of topological phase emergence on material parameters and structural conditions.

It was also recognized that numerical simulation is not merely a computational tool but an iterative research process involving hypothesis formulation, calculation, interpretation, and model refinement. The importance of critically analyzing results in light of theoretical assumptions and model limitations was clearly understood.

On the other hand, several challenges remain. The $k \cdot p$ method used in this study is an effective theory and may not fully capture atomistic interactions or impurity effects. Additionally, uncertainties in material parameters require more systematic evaluation. Future work will involve validation using more advanced models, such as first-principles calculations, and direct comparison with experimental results to further deepen the integration of simulation and experiment.

【References】

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