Kwansei Gakuin University
Report of Research Outcome

2024/03/15

To President

Department : Science and Technology
Position : Postdoctoral fellow
Name : PHAN THANH HUYEN

I report the outcome of the research as follows.

Name of the Fund/Program	□Sabbatical leave with grant □Sabbatical leave with no grant □KGU Joint Research □Individual Special Research ☒Postdoctoral fellow ※Please report by designated form as for "International Research Collaboration".
Research Theme	Theoretical Studies for Topological Design of Photonic Crystals
Research Site/Venue	Kwansei Gakuin University – Graduate School of Science and Technology
Research period	2023/10/01 ～ 2024/03/31 （6 months）

◆ **Summary of the research outcome** （**approx. 2,500 words**）

Please write down the outcomes in detail regarding the research theme above.

With the development of information and telecommunication technology, the technique of manipulating and guiding light becomes tremendously attractive. Photonic crystals (PhCs), which is the optical analog of conventional crystals, is the potential structure for this technique. There are many interesting phenomena of PhCs which can be applied for devices such as integrated optical circuit and optical switches. However, the energy-loss due to fabrication and intrinsic properties restrict the further development of photonic devices. To deal with this problem, the concept of "topology", which originates from mathematics, was applied to photonic systems. This concept can help distinguish geometry lattices by some invariant quantities during continuous deformation. Topological photonics can be understood as the cross field between PhCs and topological physics which help discover the novel phenomena of optical effects.

The purposes of our research is to theoretically design and find out new topological characteristics of PhC systems by using numerical calculations. Designing a topological PhC usually requires breaking the discrete particle symmetry of the crystals, such as time-reversal symmetry, which is not easy to achieve. Another way is to mimic the existing structure of conventional electronic crystals such as graphene, diamond cubic lattice, ...

Following the successful application of graphene and other nanoelectronics materials, the searching for new carbon materials becomes essentials. Recently, Fan, et al, has successfully synthesized the Biphenylene network (BPN). Then, A. Bafekry et al. has performed the detailed of density functional theory-based first-principles calculations to deeply study the electronic and optical properties of this material. Inspired from the initial studies of the BPN, we have studied the electronic and topological properties of the BPN by using tight binding model [1]. We also demonstrate that the topological phase transition occurs when tuning the inter- and intracellular electron hoppings. The topological edge states are induced by the non-zero Zak phase as shown in Fig. 1(b). Furthermore, we demonstrate that the exact number of edge states aligns with the number of Wannier orbital at the edge boundary. The similar argument can be used to ilustrate the existence of topological corner states in the system (Fig. 1(c) and (d)) where uncoupled Wannier orbitals are located at the corners.

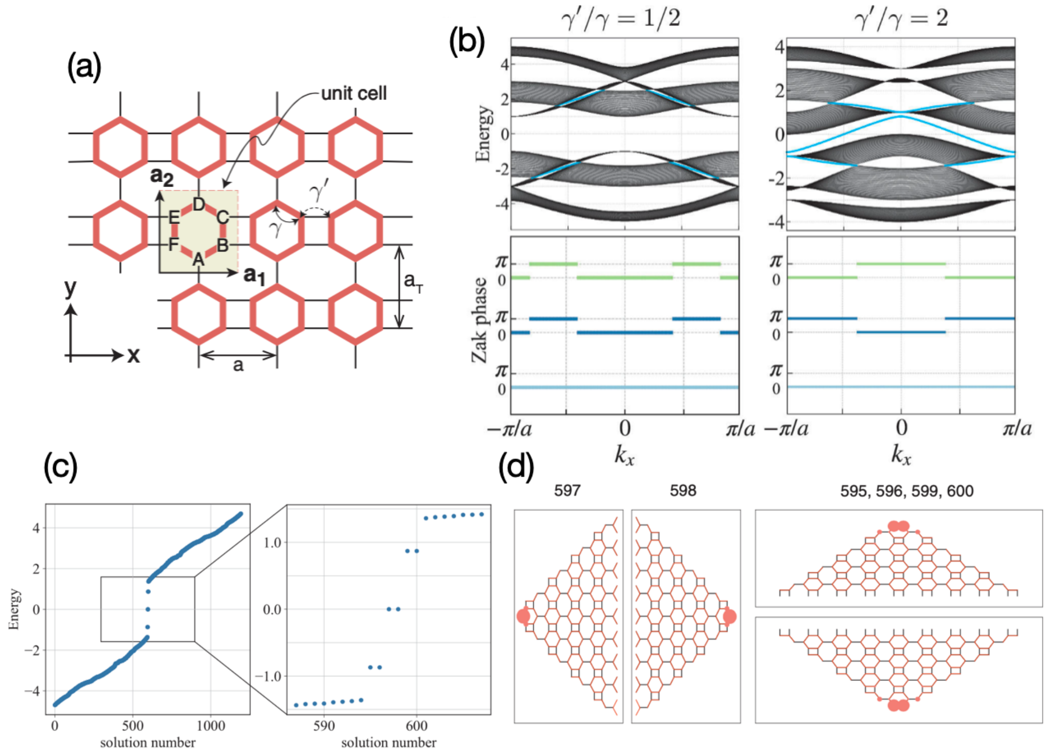

Fig. 1. (a) The lattice structure of the BPN. The shaded region is the unit cell, containing six equivalent sublattices of carbon atoms (A to F). $\boldsymbol{a}_1 = (a,0)$ *and* $\boldsymbol{a}_2 = (0,a_T)$ *are two primitive vectors. The intracellular (intercellular) hopping denoted by red (black) lines. (b) Zigzag nanoribbon edge states for different ratio of* γ'/γ*. The emergence of topological edge states is consistent with the Zak phase calculation. (c) Energy dispersion for the BPN nanoflake, which shows the isolated corner states in the band gap. (d) Wavefunctions of the topological corner states.*

Although it is very hard to tune the electron hoppings energies in the actual BPN materials, we can design a system having the topological properties of the BPN based on photonic crystals (PhCs). In our work, we also introduce a photonic crystal (PhC) structure following the BPN structure, so-called the BPN PhC [2] as shown in Fig. 2(a). We use both finite element and finite difference methods to study. This BPN PhC shows a complete band gap when $d = 1.3a_T/3$ and $r_0 = 0.2d$. By examining different ribbon structures, we obtained the topological edge states, which is localized at the zigzag and chiral edges. These edge states are induced by the non-zero Zak phase in the corresponding directions. In Fig. 2(b), the upper panel is the schematic of a ribbon with chiral edges, the middle panel present the Zak phase for the first three bands, the lower panel is the frequency dispersion of the ribbon structure. The topological edge states are observed in the complete band gap (blue line), which is consistent with the Zak phase calculation.

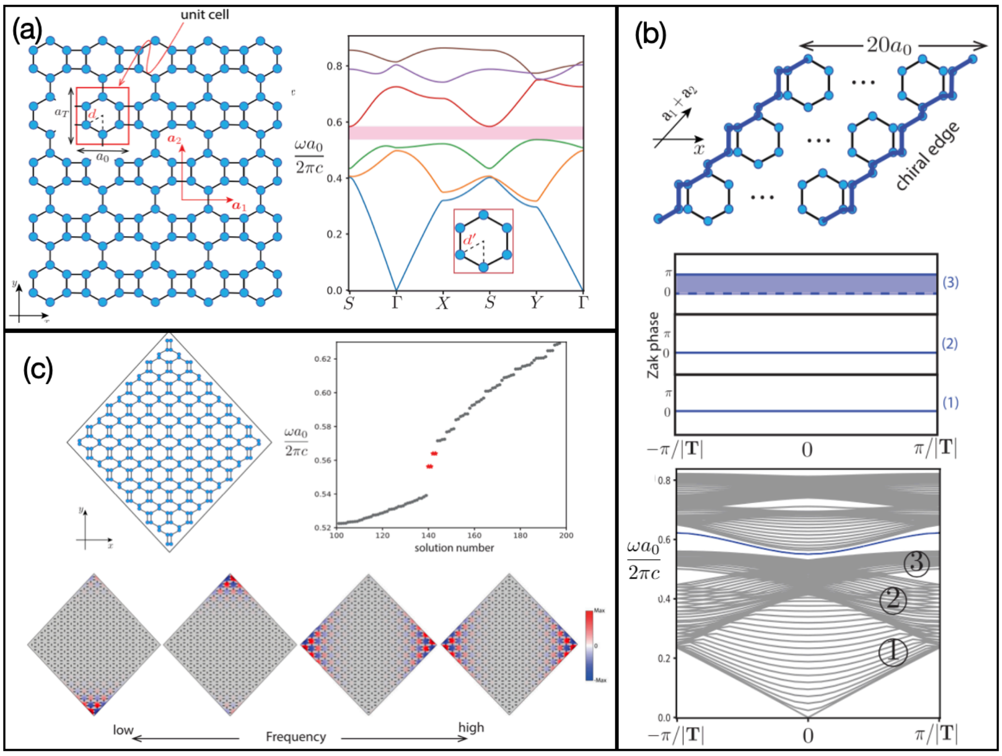

Fig. 2. (a) The left panel is the schematic of the BPN PhC. The red rectangle indicates the primitive unit cell, which contain six equivalent dielectric rods, colored by cyan. The radius of each rod is r_0, the distance between each rod and the center of the unit cell is d,). $\boldsymbol{a}_1 = (a, 0)$ and $\boldsymbol{a}_2 = (0, a_T)$ are two primitive vectors. The right panel is the photonic band structure for $d = 1.3a_T/3$, $r_0 = 0.2d$. (b) A schematic of a ribbon with chiral edges (upper panel), the corresponding Zak phase (middle panel) and the frequency dispersion (lower panel) of the ribbon. The blue line indicates the topological edge states. (c) A BPN corner structure, which contains chiral edges, the frequency dispersion of the corner structure, which shows the isolated corner states marked by red dots in the complete band gap. The field distribution for the corner states.

Similar to the studies of the BPN, here we also examine a flake structure, which contains chiral edges and four corners as shown in Fig. 2(c). The frequency dispersion show four isolated states in the band gap, labeled by re dots. These states are topological corner states, where the electromagnetic (EM) waves are localized at the corner and exponentially decay. Compared with the graphene-like PhC, the topological states in BPN-like PhC can be found without breaking the symmetry of the crystals. Our results suggest a possible way to design in-gap topological waveguide and topological confinement of EM waves.

We studied the electronic and photonic BPN parallelly. The results of our work on the BPN and its photonic counterpart are quite consistent and play an important role in the studies of both the BPN and the BPN PhC.

Beside the studies of the 2D systems, we also extend pur study to 3D PhC systems. 3D systems can provide various topological phenomena, as the third dimension expands the opportunities for the structural design of PhC or metamaterials. The topological states in 3D systems have been mainly studied in acoustic systems, there are so few report on the PhC with complete band gap. In our work, we numerically and theoretically study the topological properties of 3D simple cubic PhC [3] as shown in Fig. 3(a). This PhC structure show a complete band gap. We focus on examining the topological properties of the systems in this band gap. At the beginning, we report a numerical method for calculating the Zak phase of 3D PhC. The topological interface states are observed in the interface structure due to the finite different in the Zak phase between two types of unit cell. Owing to the inversion symmetry protection, the topological hinge states are found when the red unit cells are embedded inside the blue unit cells. Our research finding can be applied to the 3D control of microwave propagation for communication and is an important step towards the realization of robust 3D photonic circuits for infrared light.

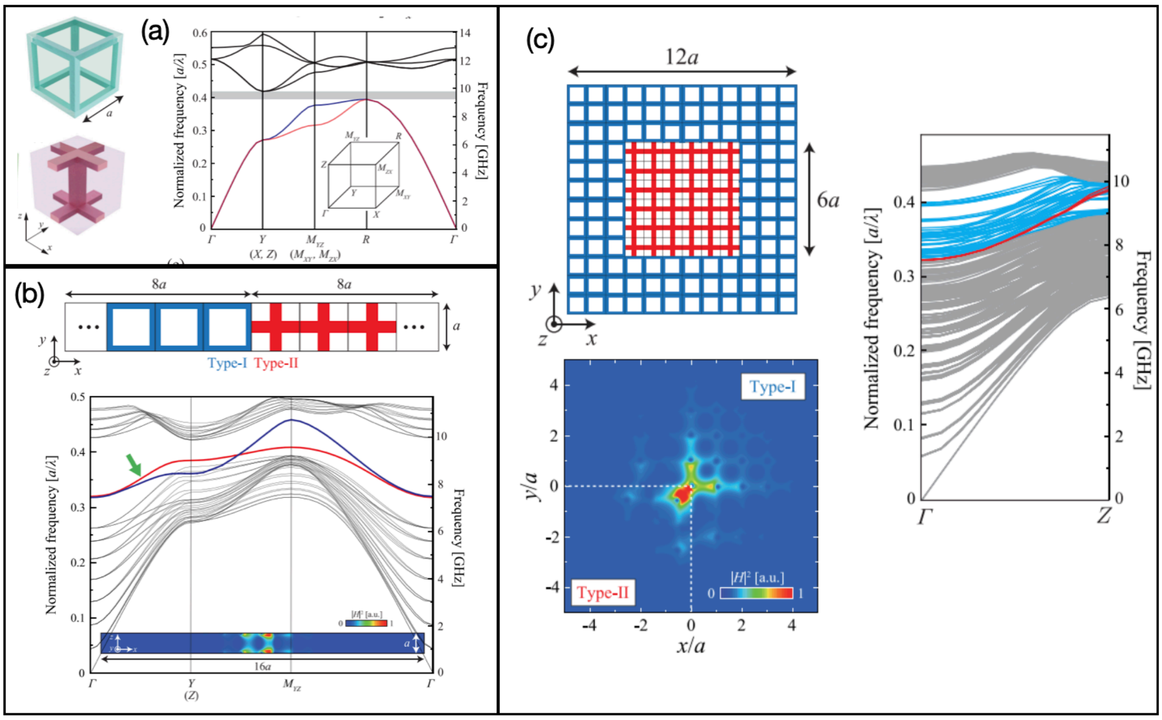

Fig. 3. (a) A schematic of two types of unit cells in simple cubic lattice and their photonic band structure, which show a complete band gap. (b) The interface structure between two types of unit cell (upper panel). The frequency dispersion is shown in the lower panel. In the complete band gap, two topological interface states are numerically observed, where the EM wave is highly localized at the interface. (c) The supercell where the red unit cells are embedded at the center and surrounded by the blue unit cells. This supercell contains 4 equivalent hinges. The bulk-interface-hinge correspondence is shown in the left panel, where bulk, interface and hingh states are colored in gray, blue and red.

In conclusion, in the last 6 months, we mainly focus on studying the topological properties of photonic crystals. Since the inversion symmetry is preserved in our systems, we use the Zak phase as a topological invariant to distinguish topological properties. In the next period, we may extend the studies to the systems without inversion symmetry or in the non-Hermitian systems.

Published papers:

[1] K. Koizumi, <u>H. T. Phan</u>, K. Nishigomi, K. Wakabayashi, Phys. Rev. B **109** 035431 (2024)
[2] <u>H. T. Phan</u>, K. Koizumi, K. Wakabayashi, Opt. Express **32** 2223-2234 (2024)
[3] S. Takahashi, Y. Ashida, <u>H. T. Phan</u>, et al., Phys. Rev. B **109** 125304 (2024)

Academic conferences:

[4] Higher Order Topological States in 3D Woodpile Photonic Crystal, H. T. Phan, et al., JST CREST Topology Joint Seminar, 9 Nov. 2023 (Komaba II Campus, University of Tokyo)
[5] <u>H. T. Phan</u>, K. Wakabayashi, Skin effect caused by point-gap topology in non-Hermitian photonic crystal, JSAP Spring Meeting 2024, Mar. 22rd, Tokyo City University.

Deadline：Within two months after finishing the research period.

Sabbatical leave with grant: Submit this report to President with confirmation by the dean of school you belong to.

※Postdoctoral fellow is required to submit this report with confirmation by the dean of graduate school before the end of employment period.

Where to submit：Organization for Research and Development and Outreach (NUC)

◆ We put this report on the web of KGU. If there is any problem about it because of difficulties on your research, please let us know.