

Research Article

Band Gap Engineering and Light Localization in Si and InP Based Three-dimensional Photonic Crystals

Fairuz Anika Salwa* , Jahirul Islam Khandaker, Mohammad Mominur Rahman, Muhammad Obaidur Rahman, Md. Abdul Mannan Chowdhury

Department of Physics, Jahangirnagar University, Dhaka, Bangladesh

Abstract

We demonstrated photonic band diagrams of three-dimensional photonic crystals composed of InP and Si for four different lattice types:- face-centered cubic (FCC), inverse opal, woodpile, and diamond structures, making 12 combinations. The Si-based FCC and inverse opal lattices exhibited no photonic band gaps (PBGs). Then, the InP-based inverse opal demonstrated small, significant 1% PBGs. After that the woodpile lattices of dielectric rods in air and diamond lattices of air voids in dielectric for both InP and Si showed large complete PBGS, enabling better photon control. A point defect was introduced in the inverse opal lattice of air voids in Si and InP background. The Si lattice didn't have a cavity mode, as it had no PBGs. The InP inverse opal lattice localized light effectively within its defect cavity using its 1% PBG, enabling it to act as a resonator and reflector. Light emission was inhibited in the surrounding photonic crystal region, as it was trapped in the defect cavity. The results obtained here are an important step towards the complete control of photons in photonic crystals.

Keywords

Photonic Band Gap (PBG), Face Centered Cubic (FCC) Lattice, Three-dimensional (3D), Photonic Crystal (PC)

1. Introduction

A three-dimensional photonic crystal is an optical nanostructure with a periodic variation in its refractive index in three dimensions, on a length scale in the order of the wavelength of light they are intended to manipulate. It can control light along all three axes incident at any angle [1-4]. Therefore, the crystal has an omnidirectional photonic band gap and allows for more complex light confinement in three-dimensions. This property allows the three-dimensional photonic crystal to control spontaneous emission [5, 6] and therefore can be used for optical applications such as frequency selection in light emitting diodes [7, 8], antenna application [9] and enhanced absorption for solar energy conversion [10]. Light can be

trapped in a three-dimensional photonic crystal defect as in two dimensions, but with the additional capability to localize light in all three dimensions. Defects in photonic crystals can localize light modes. It is trapped in all three dimensions.

This periodic variation in refractive index is achieved using a structure formed from two materials, typically a dielectric and air. As X-rays are scattered from atoms within a crystalline solid, the light waves are scattered from the periodic structure. The periodic nature of the crystal leads to coherent scattering in certain directions, as determined by the particular crystal symmetry, with an intensity dependent on the constituent material properties [11]. The dispersion relation or band structure is used to analyze

*Corresponding author: 3159anika@juniv.edu (Fairuz Anika Salwa)

Received: 29 July 2025; **Accepted:** 14 August 2025; **Published:** 29 August 2025



Copyright: © The Author(s), 2025. Published by Science Publishing Group. This is an **Open Access** article, distributed under the terms of the Creative Commons Attribution 4.0 License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution and reproduction in any medium, provided the original work is properly cited.

the properties of photonic crystals and determine whether photonic band gaps or pseudo photonic band gaps in a three dimensional photonic crystal are present. In case of three-dimensional photonic crystals, TE and TM band structures overlap with each other. We define this as the *hybrid band structure* [29].

The study of leaky modes and cavity resonances is one of the most important applications of time-domain analysis in present-day electromagnetics. In photonic crystal cavities, light cannot be trapped indefinitely. Instead, it leaks away, either because the confinement is imperfect or through unavoidable scattering losses. In such systems, the states in which energy is stored in the cavity are not true modes of the system, but finite-lifetime resonances. In the event that a given spectral resonance is reasonably isolated from any others, the stored energy decays exponentially in time and exhibits a Lorentzian line profile.

The mode profile itself can be found via a Fourier analysis during a FullWAVE simulation. The rate at which energy is lost is frequently characterized by the quality factor (Q) [12-16]. Mathematically:

$$Q = 2\pi \frac{\text{Stored energy}}{\text{Energy lost per oscillation}} = \frac{2\pi\nu}{\alpha}$$

Where ν is the stored energy and α is the energy lost per oscillation.

We investigated the photonic band gaps for face centered cubic (fcc), inverse opals, woodpile structures, and diamond structures for two different materials namely Silicon (Si) and Indium phosphide (InP). All the simulations were done using the RSoft Synopsis software, BandSolve (the plane-wave expansion method) and FullWAVE (the finite-difference time domain method), version 2023.03. Photonic band gaps were calculated using PWE, and then defect modes were calculated using FDTD. Susumu Noda [36] showed the emission spectra of a 3D PC and

its defect mode, but he did not calculate the photonic band gaps. Again, the frequency spectrum and the wavelength spectrum of the defect structure was not shown. Here we demonstrated the photonic band structures of the 3D PC first, then introduced a defect, and calculated its Q value. We found a high Q defect cavity, in comparison to ref. [12]. The quality factor, which directly sets the energy-decay rate and spectral bandwidth, also governs the efficiency of nonlinear processes and modifies spontaneous-emission rates of nearby quantum emitters; furthermore, Q is widely used to parameterize temporal coupled-mode theory (CMT) models, enabling efficient prediction of linear and complex nonlinear resonant responses that would otherwise demand costly nonlinear full-wave simulations.

2. Methodology

2.1. The Plane-wave Expansion (PWE) Method

The master equations for the electric field and that for the magnetic field are given by:

$$\hat{L}_E E(r) \equiv \frac{1}{\epsilon(r)} \nabla \times \{\nabla \times E(r)\} = \frac{\omega^2}{c^2} E(r), \quad (1)$$

$$\hat{L}_H H(r) \equiv \nabla \times \left\{ \frac{1}{\epsilon(r)} \nabla \times H(r) \right\} = \frac{\omega^2}{c^2} H(r), \quad (2)$$

where, the two differential operators $\hat{L}_E$ and $\hat{L}_H$ are defined by the first equality in each of the above equations.

Using Bloch's theorem solve these equations, we obtain the following eigenvalue equations for the expansion coefficients $E_{kn}(G)$ and $H_{kn}(G)$ in the reciprocal space [17].

$$-\sum_{G'} \kappa(G - G') (k + G') \times \{(k + G') \times E_{kn}(G')\} = \frac{\omega_{kn}^2}{c^2} E_{kn}(G), \quad (3)$$

$$-\sum_{G'} \kappa(G - G') (k + G) \times \{(k + G') \times H_{kn}(G')\} = \frac{\omega_{kn}^2}{c^2} H_{kn}(G). \quad (4)$$

This numerical method is called the plane-wave expansion method. By solving one of these two sets of equations (3) and (4) numerically, we can obtain the dispersion relation of the eigenmodes, or the photonic band structure [18, 19].

2.2. The Finite-difference Time Domain (FDTD) Method

The Finite-Difference Time-Domain (FDTD) method is a rigorous and powerful tool for modeling PC based devices. FDTD solves Maxwell's equations directly without any physical approximation. The FDTD method solves Maxwell's equations on a mesh, called a grid. A unit cell of this grid is called a Yee cell [20]. The Yee algorithm centers its E and H components in a three-dimensional space in such a way that every E component is surrounded by four circulating H

components, and every H component is surrounded by four circulating E components. This gives a three-dimensional space being filled by an interlinked array of Faraday's law and Ampere's law contours. The Yee algorithm also centers its E and H components in time in a leapfrog arrangement. The derivatives in Maxwell's equations are replaced by finite differences that results in a system of algebraic equations which are linear on coordinates. Such a system is solved sequentially starting from initial and boundary conditions [20-22].

3. Results and Discussion

We begin by reviewing the electromagnetic band structure of the semiconductors for face centered cubic (FCC), inverse opal, woodpile and diamond structures.

The face centered cubic (fcc) lattice: The unit vectors of the FCC lattice are $A = a/2(0,1,1)$, $B = a/2(1,0,1)$, and $C = a/2(1,1,0)$, where a is the distance along the edge of the conventional cubic unit cell [23].

Here, we used the following lattice parameters:

Period ie. center to center spacing, $a = 1\mu\text{m}$,

Radius, $r = 0.354\mu\text{m}$,

Diameter, $d = 0.708\mu\text{m}$.

Filling fraction which is defined as the fraction of total volume of the unit cell occupied by the dielectric medium is,

$$f = \frac{4 \times \frac{4}{3}\pi r^3}{(2 \times \sqrt{2}r)^3} \times 100\% = 0.74\% \quad (5)$$

3.1. The Face Centered Cubic (FCC) Lattice of Silicon (Si) Spheres in Air Background

We designed a 3D FCC lattice of Silicon spheres (refractive index, $n_1 = 3.6$ at optical wavelength) embedded in air background with refractive index of $n_2 = 1$ [24] as shown in figure 1. The first Brillouin zone and (c) the simulation domain of this lattice is also shown in figure 1(b) and 1(c) respectively.

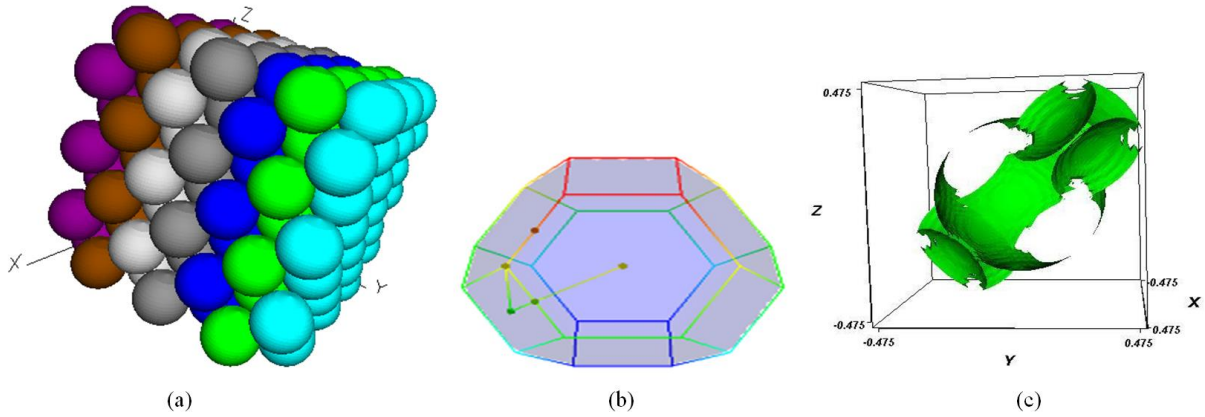


Figure 1. (a) A three-dimensional face centered cubic (fcc) photonic crystal. The crystal is made of Silicon (Si) spheres embedded in air background. (b) The first Brillouin zone and (c) the simulation domain of this lattice.

Hybrid Band Structure of the face centered cubic (fcc) lattice of Si spheres in air background

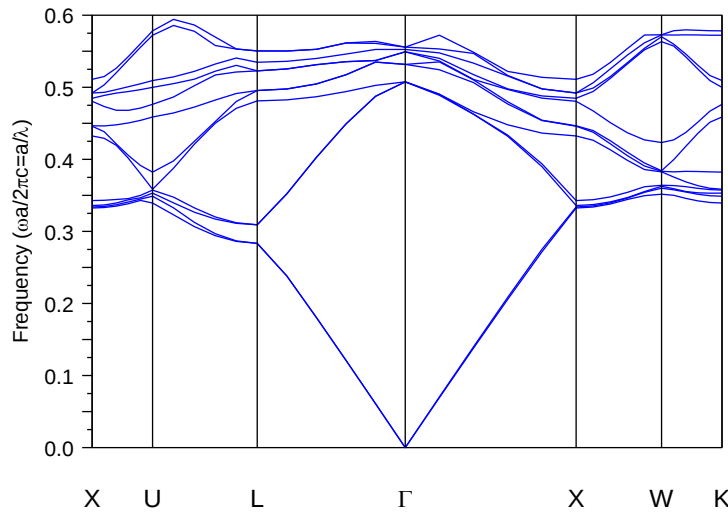


Figure 2. The hybrid band structure of the face centered cubic (fcc) lattice of Si spheres in air background.

The photonic band diagram for this structure for both TE and TM polarizations for this structure is plotted in figure 2. Twelve bands were plotted. The plane wave expansion method was implemented in modelling and simulating this band structure. No hybrid band gap occurred in this case.

The inverse opal: We found no complete band gap for the fcc lattice of dielectric spheres as shown in figure 2. Rather

we found some pseudo gaps between 2nd and 3rd bands, 4th and 5th bands, 6th and 7th bands, 7th and 8th bands and 10th and 11th bands. These gaps are important for appearing beautiful colours in opal gems [25-28]. However, the inverse structure of face centered cubic (fcc) air pores in high dielectric background is called the inverse opal [29]. The inverse opals have complete band gap.

3.2. The Inverse Opal Lattice of Air Spheres in Si Background

We reversed the fcc lattice by inserting air voids in Si back-

ground, all the lattice parameters remain same as before. The resulting photonic band diagram is shown in figure 3. No hybrid band gap was found in this case too as shown in figure 3.

Hybrid Band Structure of the face centered cubic (fcc) lattice of air spheres in Si background

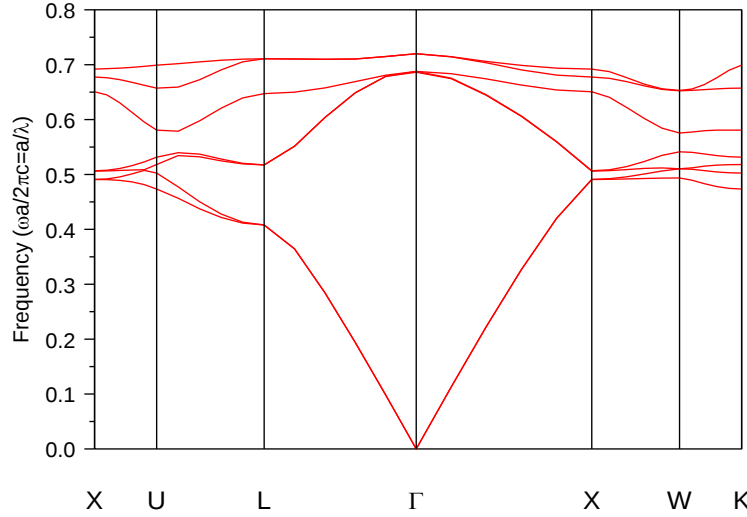


Figure 3. The hybrid band structure of the face centered cubic (fcc) lattice of air spheres in Si background.

3.3. The Face Centered Cubic (FCC) Lattice of InP Spheres in Air Background

Hybrid Band Structure of the face centered cubic (fcc) lattice of InP spheres in air background

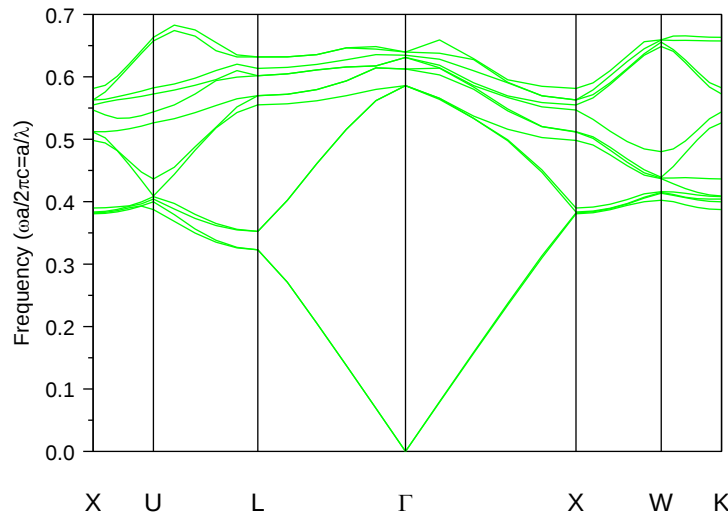


Figure 4. The hybrid band structure of the face centered cubic (fcc) lattice of InP spheres in air background.

We designed a three-dimensional (3D) FCC lattice in the Rsoft CAD layout which was composed of indium phosphide (InP) (refractive index, $n_1 = 3.156$ [24] at optical wavelength) spheres embedded in an air background with refractive index $n_2 = 1$. The crystal was periodic along the all three directions. We found no PBG for this structure also as shown in figure 4.

3.4. The Inverse Opal Lattice of Air Voids in InP Background

We designed a three-dimensional (3D) inverse opal structure in the Rsoft CAD layout which was composed of air spheres embedded in indium phosphide (InP) background.

The crystal was periodic along the all three directions. We found a small PBG for this structure as shown in figure 5.

Hybrid Band Structure of the face centered cubic (fcc) lattice of air voids in InP background

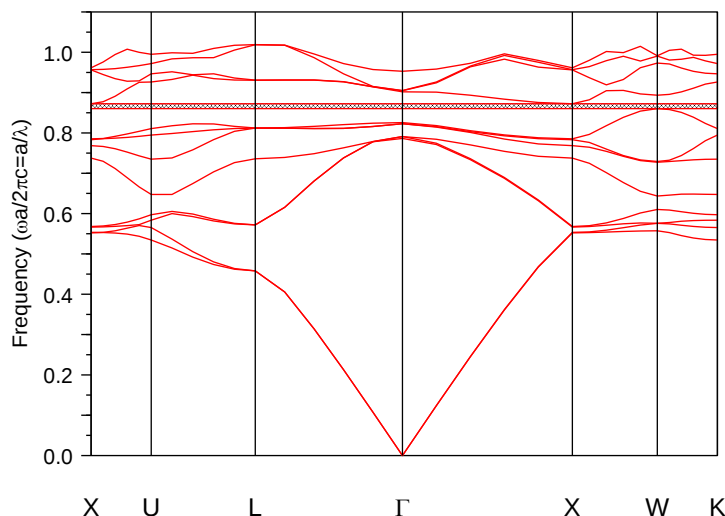


Figure 5. The hybrid Band Structure of the face centered cubic (fcc) lattice of air voids in InP background.

The band-gap width, mid-gap frequency, gap-midgap ratio and gap percentage for this structure are given in table 1.

Table 1. Photonic Band Gap Data for 3D fcc lattice of air voids in InP background.

$\frac{\omega a}{2\pi c}$	The mid-gap frequency (ω_m)	Band-gap width ($\Delta\omega$)	Gap-midgap ratio ($\Delta\omega/\omega_m$)	Gap percentage (%)
0.86 - 0.87	0.866	0.012	1.39e-02	1.39

4. The Woodpile Structure

The woodpile crystal structure is a stack of dielectric logs with alternating orthogonal orientations. The dielectric logs are generally rectangular in shape.

The simplest woodpile-like stack would be a *ABAB...* sequence, where *A* denotes one log orientation and *B* denotes the orthogonal orientation. But, this sequence does not produce a significant gap. Instead, it turns out that a four-layer *ABCDABCD...* sequence is better, in which *C* and *D* are layers with the same orientation as *A* and *B*, but are offset by half of the horizontal spacing [30, 31], as illustrated in figure 6. This structure is made of layers of dielectric rods with a stacking sequence that repeat itself every four layers with a repeat distance of *c*. Within each layer, the rods are arranged with their axes parallel and separated by a distance, *d*. The orientation of the axes are rotated by 90° between adjacent layers.

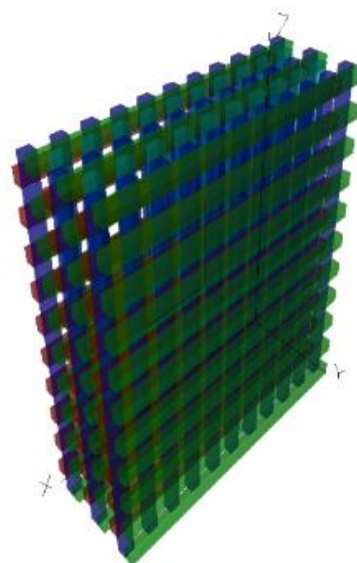


Figure 6. Electron-microscope image of a “woodpile” photonic crystal.

In general the woodpile lattice is a face-centered tetragonal or FCT lattice. This can be considered as an FCC lattice that has been rotated and stretched in the vertical (y) direction. If a is the lattice constant of the conventional cubic cell, then $a = \sqrt{2}d$, where d is the in-plane rod distance. The filling fraction [32], f for this lattice is defined by:

$$f = \frac{w}{d}. \quad (6)$$

where, w is the rod width and d is the in-plane rod distance.

The woodpile crystal is the first three-dimensional photonic crystal with a complete gap that can be fabricated on micron scales, for light at infrared wavelengths. This crystal structure was first proposed independently by Söğüt and Dowling [33] and Ho et al. [34]. It was named as a *woodpile* structure by Söğüt and Dowling [33].

The main advantage of the woodpile crystal is that the woodpile crystal can be fabricated as a sequence of layers deposited and patterned by lithographic techniques developed for the semiconductor electronics industry.

In our simulation, we used period, $a=1\mu\text{m}$, rod width, $w = 0.266 \mu\text{m}$, rod height, $h = 0.305 \mu\text{m}$, the four layer repeat distance, $c = 1.22 \mu\text{m}$, the in-plane rod distance, $d = 0.707 \mu\text{m}$. So, the filling fraction was, $f = 37.62\%$.

We designed a three-dimensional (3D) woodpile lattice in

the Rsoft CAD layout which was composed of rectangular Si rods ($n_1 = 3.6$) embedded in air background with refractive index of $n_2 = 1$. The first Brillouin zone of this lattice is shown in figure 7.

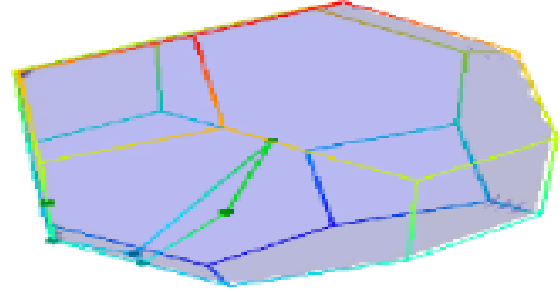


Figure 7. The first Brillouin zone for this lattice.

The photonic band diagram for this structure as in figure 8 shows that there is a large band gap between the 2nd and 3rd bands with a gap-midgap ratio of 20.37%. Band structures for an infinite inverse woodpile crystal made of silicon and air showed 25% PBG as computed by C. P. Mavidis et. al. [34].

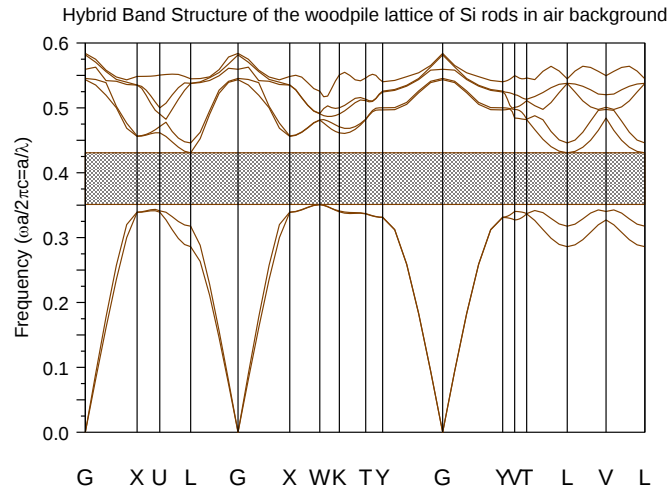


Figure 8. The hybrid Band Structure of the woodpile lattice of Si rods in air background.

The band-gap width, mid-gap frequency, gap-midgap ratio and gap percentage for this structure are given in table 2.

Table 2. Photonic Band Gap Data for the 3D Woodpile Lattice of silicon (Si) Rods in Air Background.

$\frac{\omega a}{2\pi c}$	The mid-gap frequency (ω_m)	Band-gap width ($\Delta\omega$)	Gap-midgap ratio ($\Delta\omega/\omega_m$)	Gap percentage (%)
0.35 - 0.43	0.391	0.08	0.204	20.37

4.1. The Woodpile Lattice of Air in Si Background

We designed a three-dimensional (3D) woodpile lattice in

the Rsoft CAD layout which was composed of rectangular air in Si background.

We found no PBG for this structure as shown in figure 9.

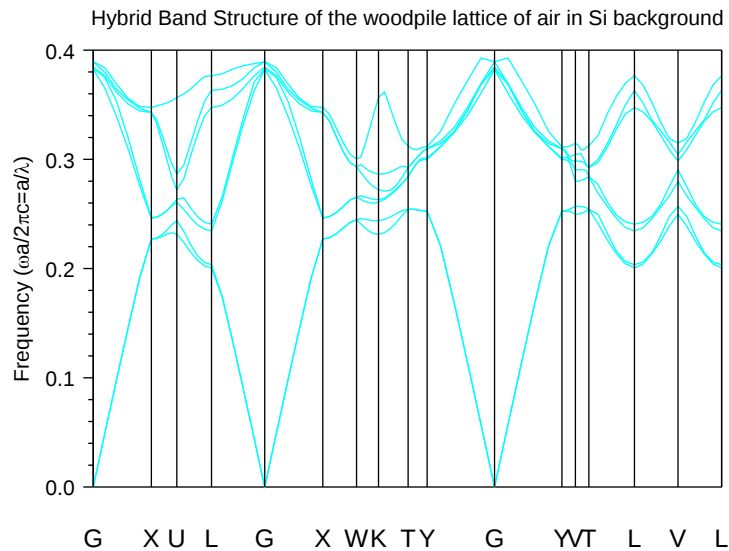


Figure 9. Hybrid Band Structure of the woodpile lattice of air in Si background.

4.2. The Woodpile Lattice of InP Rods in Air Background

We designed a three-dimensional (3D) woodpile lattice in the Rsoft CAD layout which was composed of rectangular InP

embedded in air background.

The hybrid band diagram for this structure is plotted in figure 10. Six bands were plotted. The plane wave expansion method was implemented in modelling and simulating this band structure. There is a complete band gap between the second and third band with a gap-midgap ratio of 15.34%.

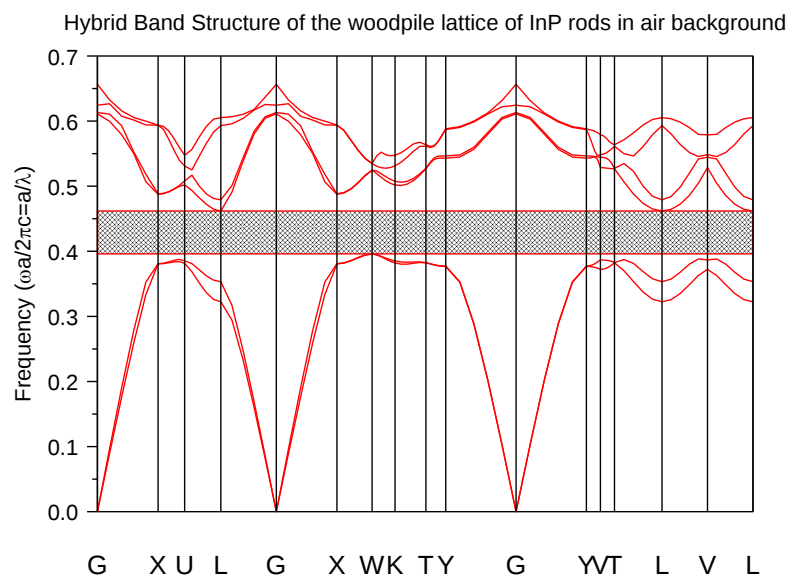


Figure 10. The hybrid band structure of the woodpile lattice of InP rods in air background.

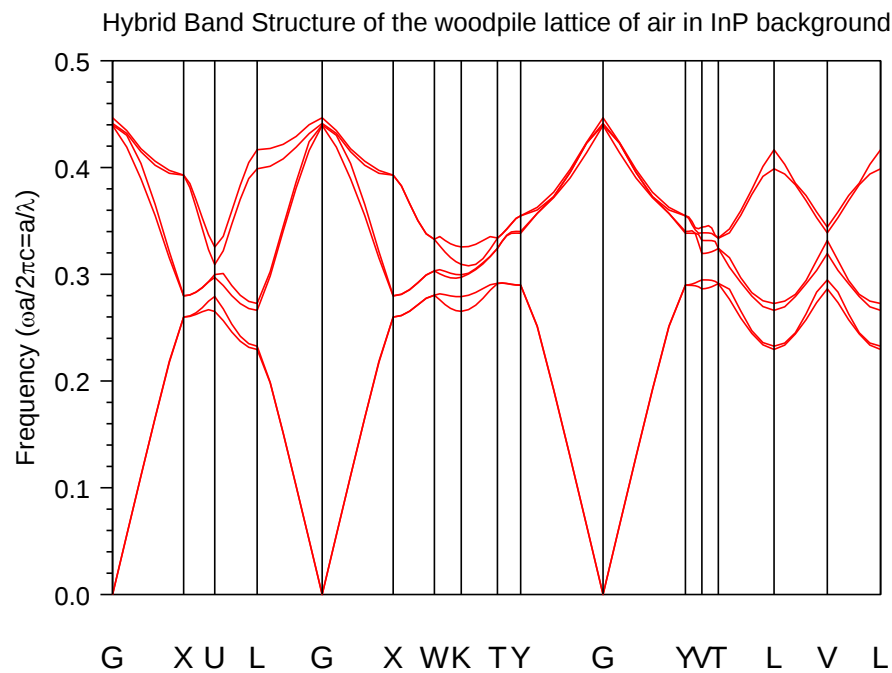
The band-gap width, mid-gap frequency, gap-midgap ratio and gap percentage for this structure are given in table 3.

Table 3. Photonic Band Gap Data for the 3D Woodpile Lattice of Indium Phosphide (InP) Rods in Air Background.

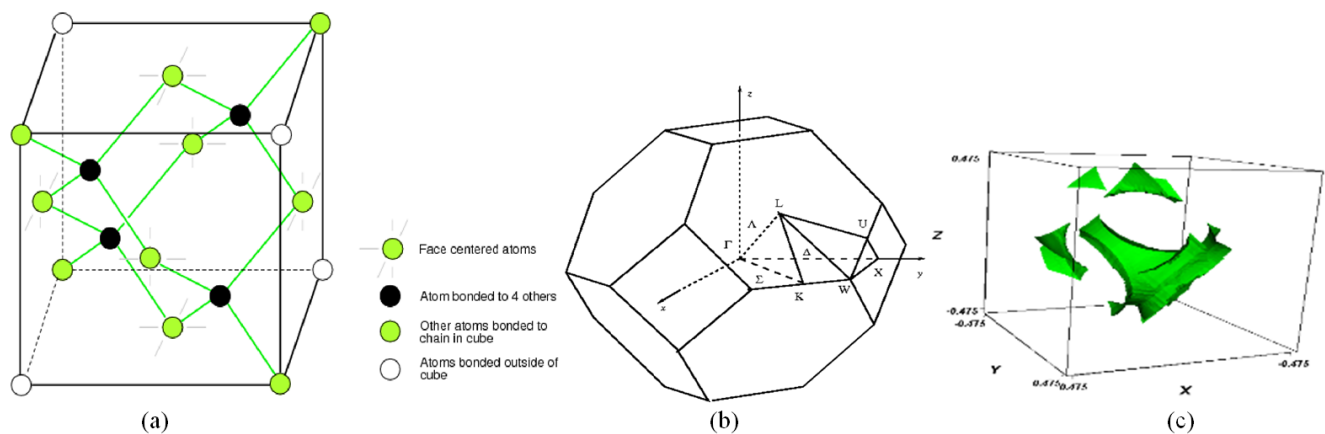
$\frac{\omega a}{2\pi c}$	The mid-gap frequency (ω_m)	Band-gap width ($\Delta\omega$)	Gap-midgap ratio ($\Delta\omega/\omega_m$)	Gap percentage (%)
0.39 - 0.46	0.43	0.07	0.153	15.34

4.3. The Woodpile Lattice of Air in InP Background

We designed a three-dimensional (3D) woodpile lattice in the Rsoft CAD layout which was composed of air embedded in rectangular InP background. The woodpile lattice of air in InP background has no PBG as shown in figure 11.

**Figure 11.** The hybrid Band Structure of the woodpile lattice of air in InP background.

5. The Diamond Structure

**Figure 12.** (a) The unit cell of a diamond crystal lattice and (b) k-Path of the first Brillouin zone and (c) the simulation domain for this lattice.

The diamond crystal lattice is a face-centered cubic (FCC) lattice with two spherical atoms in the unit cell as shown in figure 12. Here, four atoms (black) are bonded to four others within the volume of the cell. Six atoms fall on the middle of each of the six cube faces, showing two bonds. Out of eight cube corners, four atoms bond to an atom within the cube. The other four bond to adjacent cubes of the crystal.

Assuming the length of the side of the unit cell is a , the primitive lattice vectors are, $a_1 = (0, 1, 1)a/2$, $a_2 = (1, 0, 1)a/2$ and $a_3 = (1, 1, 0)a/2$ with atom positions $(0,0,0)a$ and $(1/4, 1/4, 1/4)a$. Basis reciprocal lattice vectors are $b_1 = (-1, 1, 1)2\pi/a$, $b_2 = (1, -1, 1)2\pi/a$ and $b_3 = (1, 1, -1)2\pi/a$. The filling fraction, f for this lattice is defined by [15]:

$$f = 2 \times \frac{4\pi r^3}{3a^3} \quad (7)$$

where, r is the radius of the sphere.

Here, $r = 0.325\mu\text{m}$, diameter of the spheres, $d = 0.65\mu\text{m}$, $a = 1\mu\text{m}$.

5.1. The Diamond Lattice of Si Spheres in Air Background

We designed a three-dimensional (3D) diamond lattice in the Rsoft CAD layout which was composed of spherical Si embedded in air background as shown in figure 12(a). Here, period, $a = 1\mu\text{m}$, radius, $r = 0.325\mu\text{m}$, diameter, $d = 0.65\mu\text{m}$.

It has no PBG as shown in figure 13(a). But when we varied the radius, a small PBG appeared at $r = 0.2\mu\text{m}$ as shown in the gap map of figure 12(b). All the gaps seals up at $r = 0.28\mu\text{m}$. With increasing radius r , the gap size increases first and then decreases, but the gaps are decreased in frequency as shown in figure 13(c) and (d).

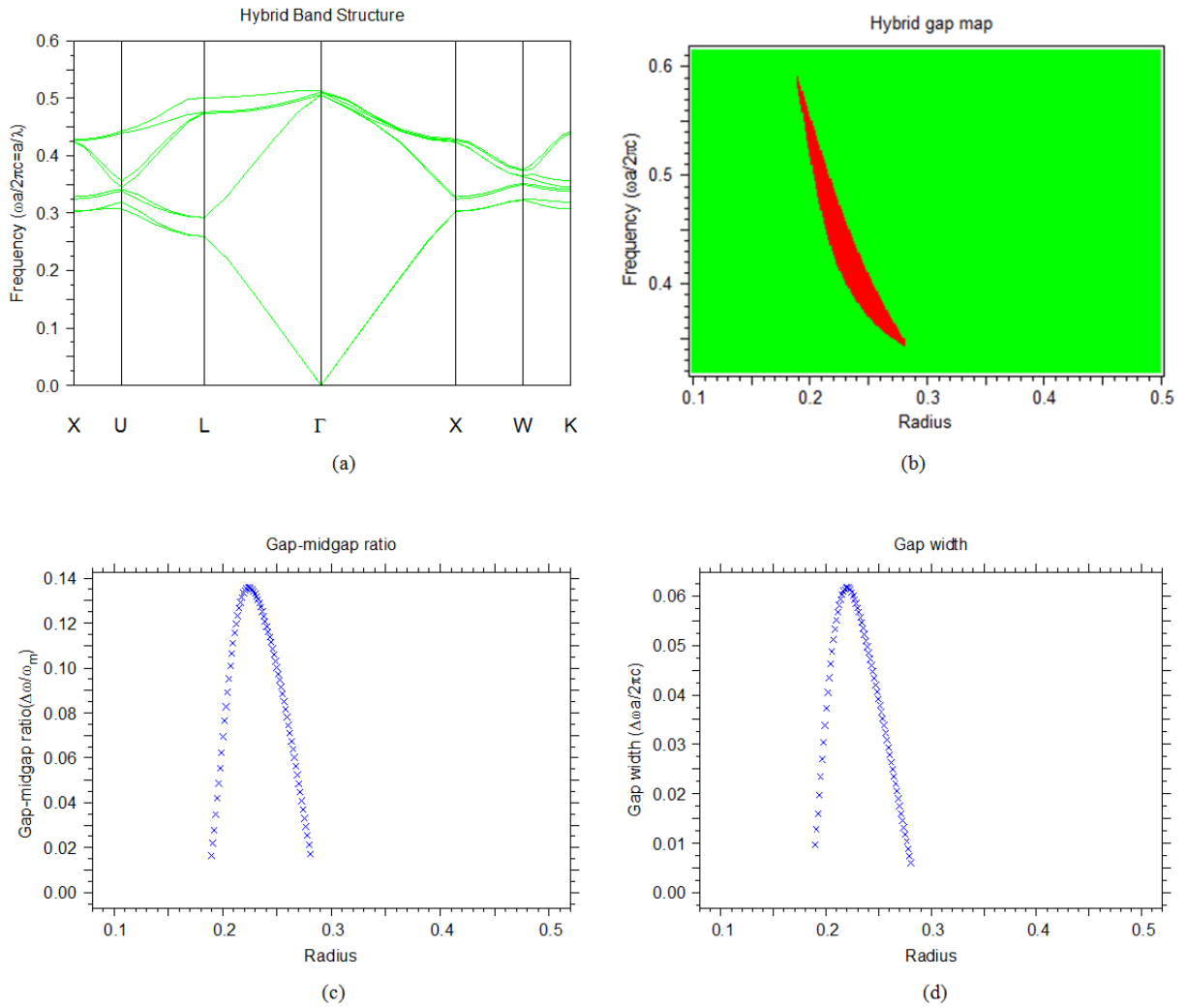


Figure 13. (a) Hybrid Band Structure, (b) hybrid gap map, (c) gap-midgap ratio and (d) gap width of the diamond lattice of Si spheres in air background.

5.2. The Diamond Lattice of Air Spheres in Si Background

We designed a three-dimensional (3D) diamond lattice in the Rsoft CAD layout which was composed of air spheres embedded in Si background. Figure 14(a) shows that the diamond lattice of air spheres in Si background has a large PBG of 28.13%. From the gap map of figure 14(b), we see

that the gaps are increased in frequency with radius r . A small PBG formed at $r = 0.227\mu\text{m}$ and sealed up at $r = 0.374\mu\text{m}$, as shown in the gap map of figure 14(b). Figure 14(c) and (d) shows that the gap size curve has a positive slope upto $r = 0.33\mu\text{m}$ and then a negative slope. The band-gap width, mid-gap frequency, gap-midgap ratio and gap percentage for this structure are given in table 4.

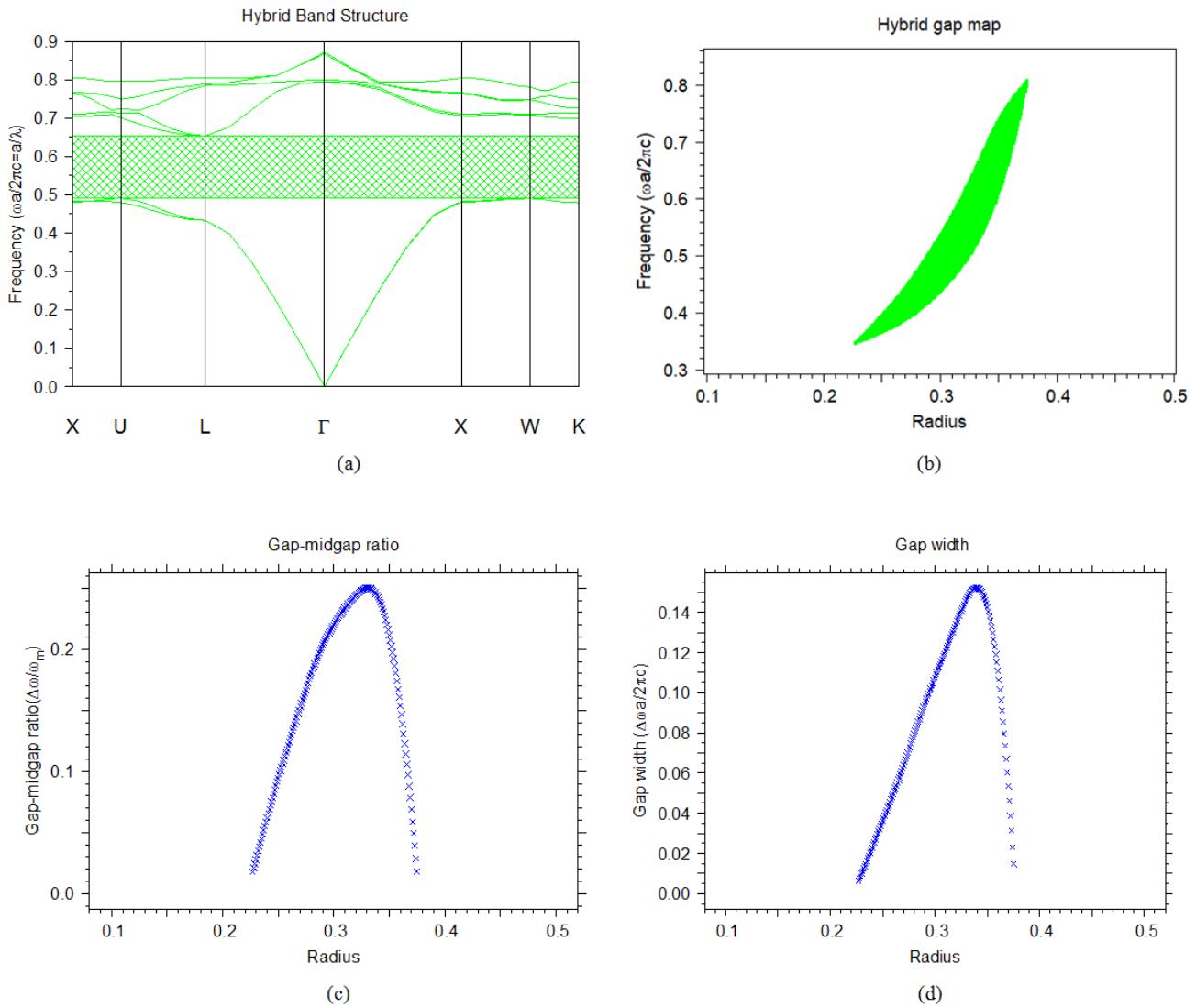


Figure 14. (a) Hybrid Band Structure, (b) hybrid gap map, (c) gap-midgap ratio and (d) gap width of the diamond lattice of air spheres in Si background.

Table 4. Photonic Band Gap Data for 3D Diamond Lattice of Air spheres in Silicon (Si).

$\frac{\omega a}{2\pi c}$	The mid-gap frequency (ω_m)	Band-gap width ($\Delta\omega$)	Gap-midgap ratio ($\Delta\omega/\omega_m$)	Gap percentage (%)
0.492 - 0.653	0.57	0.16	0.28	28.13

5.3. The Diamond Lattice of InP Spheres in Air Background

We designed a three-dimensional (3D) diamond lattice in the Rsoft CAD layout which was composed of spherical InP embedded in air background.

The hybrid band structure of figure 15(a) shows that the

diamond lattice of InP spheres in air background has no PBG. We performed a radius scan of this lattice from $r = 0.1\mu\text{m}$ to $r = 0.5\mu\text{m}$, as shown in figure 15(b). A PBG appears at $r = 0.19\mu\text{m}$ and disappears at $r = 0.28\mu\text{m}$. The gap size curve of figure 14(c) and (d) shows that a maximum PBG of 5% occurred at $r = 0.223\mu\text{m}$.

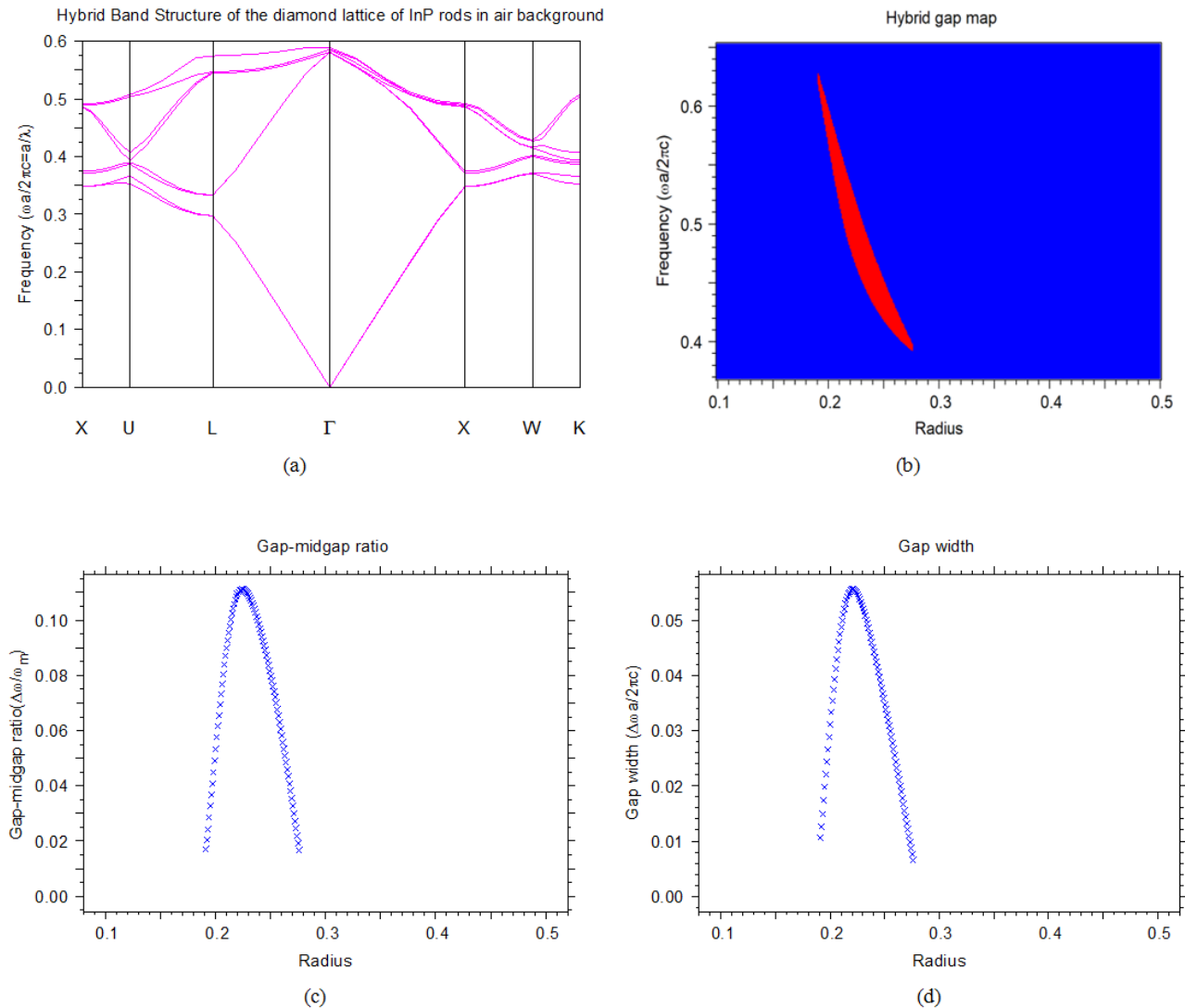


Figure 15. (a) Hybrid Band Structure, (b) hybrid gap map, (c) gap-midgap ratio and (d) gap width of of the diamond lattice of InP spheres in air background.

5.4. The Diamond Lattice of Air Spheres in InP Background

Table 5. Photonic Band Gap Data for the Three-Dimensional (3D) diamond lattice of air spheres in InP background.

$\frac{\omega a}{2\pi c}$	The mid-gap frequency (ω_m)	Band-gap width ($\Delta\omega$)	Gap-midgap ratio ($\Delta\omega / \omega_m$)	Gap percentage (%)
0.56 - 0.68	0. 62	0.12	0.189	18.85

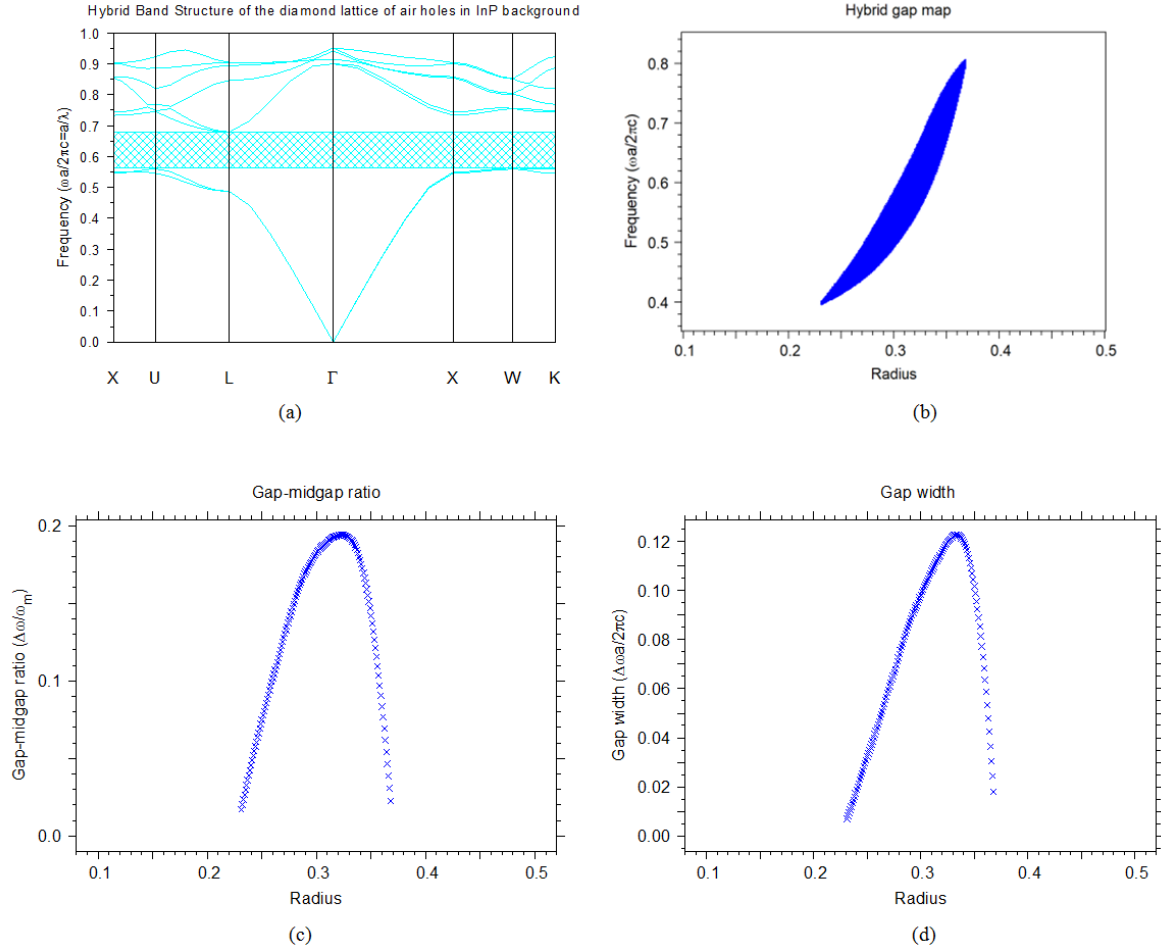


Figure 16. (a) Hybrid Band Structure, (b) hybrid gap map, (c) gap-midgap ratio and (d) gap width of of the diamond lattice of air spheres in InP background.

We designed a three-dimensional (3D) diamond lattice in the Rsoft CAD layout which was composed of air embedded in spherical InP background. Figure 16(a) shows that this structure had a large PBG having gap-midgap ratio of 0.189. It

has a maximum gap of 19.5% at $r = 0.328\mu\text{m}$. The band-gap width, mid-gap frequency, gap-midgap ratio and gap percentage for this structure are given in table 5.

6. Localization at a Point Defect

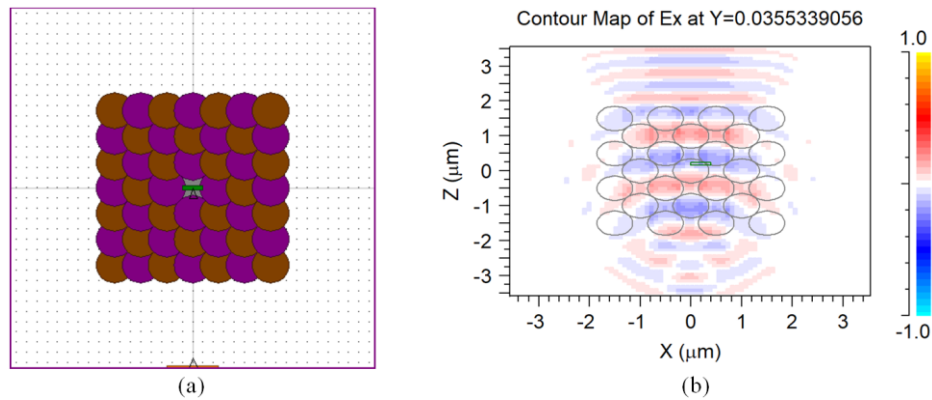


Figure 17. (a) A 3D point defect introduced by the central missing air void in a solid medium, (b) Light is scattered in all directions in the face centered cubic (fcc) lattice of air spheres in Si background.

Photonic band gap is the ranges of optical frequencies which are forbidden to propagate within the photonic crystal medium. This allows a photonic crystal to act as a kind of omnidirectional reflector, assuming that the band gap exists for all relevant propagation directions - ideally, for any directions in three dimensions. A photonic crystal is thus suitable for enclosing structures in order to prevent light from escaping [35]. Similarly, a photonic crystal can be used to confine light to different kinds of structures, which can be considered as some kind of intentionally introduced lattice defects.

We created a point defect in the face centered cubic (fcc) lattice of air spheres in Si background by removing an air void from the center of the xz plane, as shown in figure 17(a). We sent a continuous light wave with a gaussian envelope in time. We used $0.004\mu\text{m}$ grid size and perfectly matched layer (PML) boundary condition. The PML width was $0.5\mu\text{m}$. We consider TE polarization only. As we saw from the previous section, this structure did not exhibit a cavity mode, so light is not be

guided in this crystal, as shown in figure 17(b).

After that, we introduced a point defect by the missing air void in the xz face of the face centered cubic (fcc) lattice of air voids in InP background. All the FDTD settings were remain the same. Light is strongly localized in this defect as shown in figure 19. Because this lattice has a PBG, that is this crystal prohibits the propagation of certain wavelengths of light. A wide range of frequencies was excited ie. We used a pulsed excitation and the frequency response of the defect was measured using the FDTD method. The peaks in the response represent defect mode frequencies. We found the resonance frequency and resonant wavelength for this lattice were, $f = 0.395\mu\text{m}^{-1}$ and $\lambda = 2.48\mu\text{m}$, as shown in figure 18(a) and (b) respectively. For this reason the mode profile was calculated at $2.48\mu\text{m}$. The Q value for this cavity was calculated as $Q = 4.8959$. From figure 19, we see that the mode is trapped in the defect. In this way the defective fcc lattice of air voids in InP can act as a resonator and reflector.

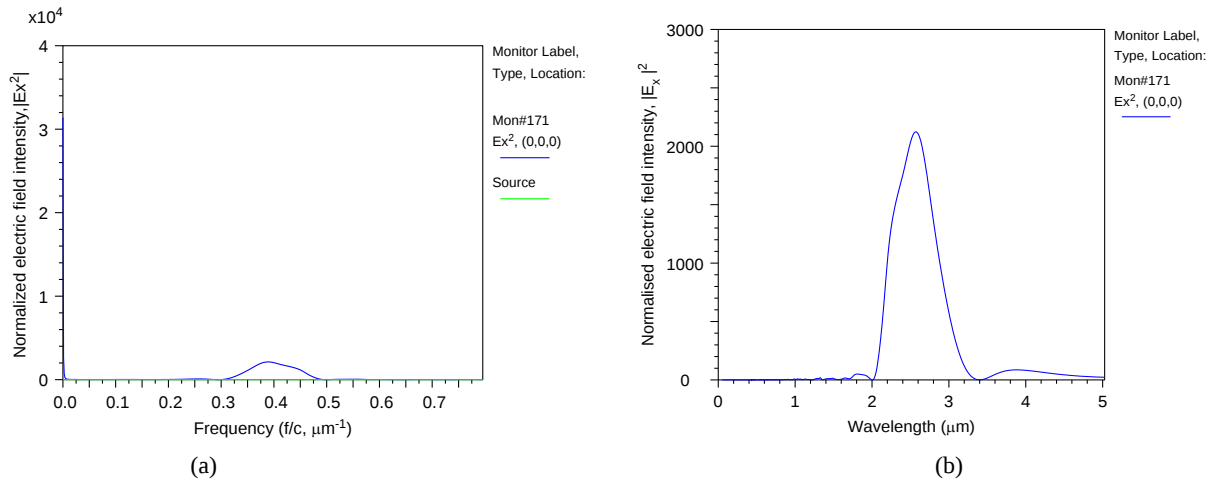


Figure 18. (a) The frequency spectrum and (b) the wavelength spectrum found from the impulse simulation of the defect structure. The peak at $0.39\mu\text{m}^{-1}$ represents a wavelength of $2.48\mu\text{m}$.

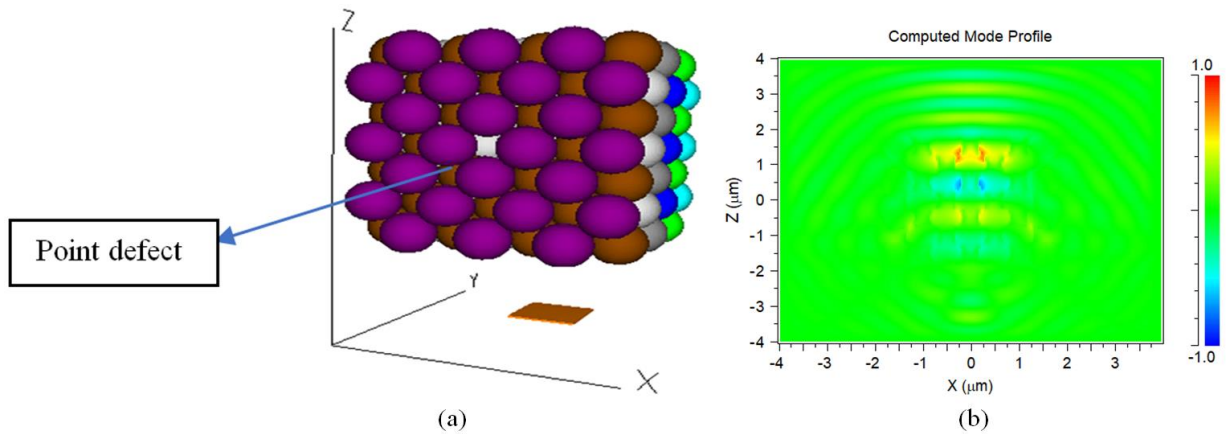


Figure 19. (a) 3D view of the point defect and (b) the computed defect mode. This is a doubly degenerate dipole state.

7. Conclusions

This study explored photonic band diagrams of three-dimensional photonic crystals composed of InP and Si for four different lattice types:- face-centered cubic (FCC), inverse opal, woodpile and diamond structures, making 12 combinations. The Si-based FCC and inverse opal lattices exhibited no photonic band gaps (PBGs), whereas the InP-based inverse opal demonstrated small PBGs. Silicon is from Group 14 (the carbon group) of the periodic table, while indium phosphide (InP) is a compound semiconductor formed from elements in Group 13 (indium) and Group 15 (phosphorus), making it a III-V semiconductor. Due to their structural difference, InP-based inverse opal exhibited PBG. The woodpile lattice of dielectric rods in air and diamond structure of air in dielectrics showed significant PBGs, enabling better photon control. From our study, we suggest that the diamond structure is the best 3D photonic crystal lattice exhibiting large photonic band gap.

We think that the high air volume in inverse opal and diamond structures contributed to better light trapping and PBG formation. Here, the diameter of the spheres was larger than the period, causing the air spheres to overlap. Both the air and the dielectric regions were connected. So, this crystal can be thought of as composed of two interpenetrating diamond lattices, one of which is composed of connected air spheres, and the other of which is composed of connected dielectric channels. Through the channels, the electric field lines can run, for the modes in the lowest bands. However, they are narrow enough that higher bands are forced out, and the corresponding frequency difference produces the large photonic band gap.

We found a smaller band-gap for the three-dimensional woodpile lattice made of dielectric rods embedded in air background than three-dimensional diamond lattice of air spheres embedded in dielectric background. Usually, a complete photonic band gap appears if the edge of the Brillouin zone has the same magnitude $|k|$ in all directions, corresponding to a spherical Brillouin zone. However, there is no three-dimensional crystal with a spherical Brillouin zone. It is generally a polygonal solid. Thus, the band gaps in different directions generally occur at different frequencies. Only the diamond lattice have nearly spherical Brillouin zone. That is why the diamond structure outperforms the woodpile in terms of PBG size.

The gap map of diamond lattice of dielectric spheres in air background shows that with increasing radius r , the gaps are decreased in frequency. On the other hand, the gap map of diamond lattice of air spheres in dielectric background shows that the gaps are increased in frequency with increasing r . At first the gap size curve has a positive slope upto they reaches a maxima and then a negative slope. We measured an optimum value of the rod radius for which maximum PBG was obtained. When the rod are almost touching to each other, all gaps are vanished.

Finally, a point defect was introduced in the inverse opal lattice of air voids in Si and InP background. The Si lattice didn't have a cavity mode. The InP inverse opal lattice lo-

calized light effectively within its defect cavity, enabling it to act as a resonator. Light emission was inhibited in the photonic crystal region, as it was trapped in the defect cavity. This PC can act as an omnidirectional reflector and resonator in optical telecommunication.

Abbreviations

FCC	Face-Centered Cubic
PBG	Photonic Band Gap
TE	Transverse Electric
TM	Transverse Magnetic
3D	Three-dimensional
PC	Photonic Crystal
Q	Quality Factor
PWE	Plane-wave Expansion Method
FDTD	Finite-Difference Time Domain Method

Acknowledgments

The authors thank the Information and Communication Technology Division (ICT- Division), Department of the Ministry of Posts, Telecommunications and Information Technology of the Government of Bangladesh, for providing the prestigious ICT fellowship 2021-22 (3rd round) and supporting this research work.

Author Contributions

Fairuz Anika Salwa: Writing – original draft

Jahirul Islam Khandaker: Writing – review & editing

Mohammad Mominur Rahman: Writing – review & editing

Muhammad Obaidur Rahman: Writing – review & editing

Md. Abdul Mannan Chowdhury: Writing – review & editing

Conflicts of Interest

The authors declare no conflicts of interest.

References

- [1] S. John, "Strong localization of photons in certain disordered dielectric superlattices," 1987, *Phys. Rev. Lett.*, vol. 58, no. 23, pp. 2486-2489.
- [2] E. Yablonovitch, "Inhibited spontaneous emission in solid-state physics and electronics," 1987, *Phys. Rev. Lett.*, vol. 58, no. 20, pp. 2059-2062.
- [3] S. John, "Photonic band gap materials: a semiconductor for light," in *4th Pacific Rim Conference on Lasers and Electro-Optics*, 2001, pp. 1-23.

- [4] R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos, "Nature of the photonic band gap: Some insights from a field analysis," 1993, *J. Opt. Soc. Am. B*, vol. 10, no. 2, p. 328.
- [5] S. Noda and F. T. Asano, "Spontaneous-emission control by photonic crystals and nanocavities," 2007, *Nat. Photonics*, vol. 1, no. 8, pp. 449-458.
- [6] S. Noda, "Photonic crystal lasers -ultimate nanolasers and broad-area coherent lasers," 2010, *J. Opt. Soc. Am. B*, vol. 27, no. 11, pp. B1-B8.
- [7] C. F. Lai, C. C. Chang, M. J. Wang, M. K. Wu; L. C., "CCT- and CRI-tuning of white light-emitting diodes using three-dimensional non-closepacked colloidal photonic crystals with photonic stop-bands," 2013, *Opt. Express*, vol. 21, S4, pp. 687-694.
- [8] Anna Starczewska and Mirosława Kępińska, "Photonic Crystal Structures for Photovoltaic Applications", 2024, *Materials*, vol. 5, 17, 1196.
- [9] A. L. Reynolds, "Explaining Photonic Band Gap Materials." [Online]. Available: <http://web.eng.gla.ac.uk/groups/opto/junkpbpg/Photonics/photonicmain.htm>
- [10] K. P. H. M, and L. S., "Integrated three-dimensional photonic nanostructures for achieving near-unity solar absorption and superhydrophobicity," 2015, *J. Appl. Phys.*, vol. 117.
- [11] Y. Aoyagi and K. Kajikawa, "Optical Properties of Advanced Materials," 2013, *Optical Properties of Advanced Materials*, vol. 168. <https://doi.org/10.1007/978-3-642-33527-3>
- [12] Thomas Christopoulos, Odysseas Tsilipakos, Georgios Sinatkas, and Emmanouil E. Kriezis, "On the calculation of the quality factor in contemporary photonic resonant structures," 2019, *Opt. Express*, vol. 27, pp. 14505-14522, <https://doi.org/10.1364/OE.27.014505>
- [13] Takashi Asano, Yoshiaki Ochi, Yasushi Takahashi, Katsuhiro Kishimoto, and Susumu Noda, "Photonic crystal nanocavity with a Q factor exceeding eleven million," 2017, *Opt. Express*, vol. 25, no. 1769-1777.
- [14] "Thomas Christopoulos, Odysseas Tsilipakos, Georgios Sinatkas, and Emmanouil E. Kriezis, "On the calculation of the quality factor in contemporary photonic resonant structures," 2019, *Opt. Express* 27, 14505-14522.
- [15] A. Daud Khan and Aimal Daud Khan, "High Q-factor photonic crystal cavities," 2015. <https://doi.org/10.1109/ICET.2015.7389173>
- [16] "Q Factor." [Online]. Available: https://www.rp-photonics.com/q_factor.html
- [17] K. Sakoda, *Optical Properties of Photonic Crystals*, Second Edi., 2004, vol. 53, no. 9. Springer. <https://doi.org/10.1017/CBO9781107415324.004>
- [18] S. Shi, C. Chen, and D. W. Prather, "Plane-wave expansion method for calculating band structure of photonic crystal slabs with perfectly matched layers," 2004, *J. Opt. Soc. Am. A*, vol. 21, no. 9, pp. 1769-1775.
- [19] W. C. Saylor, F. M. Mueller, and P. R. Villeneuve, "Augmented-plane-wave method for photonic band-gap materials," 1998, *Phys. Rev. B*, vol. 57, no. 15, pp. 8819-8822.
- [20] Z. Zhang and S. Satpathy, "Electromagnetic wave propagation in periodic structures: Bloch wave solution of Maxwell's equations," 1990, *Phys. Rev. Lett.*, vol. 65, no. 21, pp. 2650-2653.
- [21] Pietruszka, P.; Stefański, T. P.; Gulowski, J. FDTD Method for Electromagnetic Simulations in Media Described by Time-Fractional Constitutive Relations. *Appl. Sci.* 2023, 13, 10654. <https://doi.org/10.3390/app131910654>
- [22] A. Taflove and S. C. Hagness, *Computational Electrodynamics The Finite-Difference Time-Domain Method*, Third Edit. Artech House, 2005.
- [23] K. M. Leung and Y. F. Liu, "Full vector wave calculation of photonic band structures in face-centered-cubic dielectric media," 1990, *Phys. Rev. Lett.*, vol. 65, no. 21, pp. 2646-2649.
- [24] "Refractive Index. INFO, Refractive index database," [Online] Available: <https://refractiveindex.info/>
- [25] K. Xiang, H.; Yang, S.; Talukder, E.; Huang, C.; Chen, "Research and Application Progress of Inverse Opal Photonic Crystals in Photocatalysis," 2023, *Inorganics*, vol. 11, no. 337, [Online]. Available: <https://doi.org/10.3390/inorganics11080337>
- [26] X. Z. Zhu, Changqing Fang, Mengyuan Pu, Jing Song, Dong Wang, "Recent advances in photonic crystal with unique structural colors: A review," 2023, *J. Mater. Sci. Technol.*, vol. 141, pp. 78-99,, [Online]. Available: <https://doi.org/10.1016/j.jmst.2022.08.044>
- [27] C. Aguirre, E. Reguera, and A. Stein, "Tunable Colors in Opals and Inverse Opal Photonic Crystals," 2010, *Adv. Funct. Mater.*, vol. 20, no. 16, pp. 2565-2578, <https://doi.org/10.1002/adfm.201000143>
- [28] Hao Chen, Jingjiang Wei, Fei Pan, Tianyu Yuan, Yuanlai Fang, Qingyuan Wang, "Advances in Photonic Crystal Research for Structural Color", 2024, <https://doi.org/10.1002/admt.202400865>
- [29] J. J. D. Joannopoulos, S. Johnson, J. N. J. Winn, and R. R. D. Meade, *Photonic crystals: molding the flow of light*, 2008, <https://doi.org/10.1063/1.1586781>
- [30] K. A. I. L. Wijewardena Gamalath and S. E. Dissanayake, "Three Dimensional photonic crystals," 2015, *world Sci. News*, vol. 6, pp. 57-68. (Online) Available: www.worldscientificnews.com
- [31] S.-Y. Lin, J. G. Fleming, D. L. Hetherington, B. K. Smith, R. Biswas, K. M. Ho, *et al.*, "A three-dimensional photonic crystal operating at infrared wavelengths," 1998, *Nature*, vol. 394, no. 6690, pp. 251-253.
- [32] R. Iliew, C. Etrich, and F. Lederer, "Self-collimation of light in three-dimensional photonic crystals," 2005, *Opt. Express*, vol. 13, no. 18, pp. 7076-7085.
- [33] H. S. Özler and J. P. Dowling, "Photonic band calculations for woodpile structures," 1994, *J. Mod. Opt.*, vol. 41, no. 2, pp. 231-239.

- [34] K. M. Ho, C. T. Chan, C. M. Soukoulis, R. Biswas, and M. Sigalas, "Photonic band gaps in three dimensions: New layer-by-layer periodic structures," 1994, *Solid State Commun.*, vol. 89, no. 5, pp. 413-416.
- [35] Schulz, A. S., Kozon, M., Vancso, J., Huskens, J., & Vos, W. L. "Strongly inhibited spontaneous emission of PbS quantum dots covalently bound to 3D silicon photonic band gap crystals," 2024, *The Journal of physical chemistry C*, vol. 22, 128, 9142-9153. <https://doi.org/10.1021/acs.jpcc.4c01541>
- [36] Susumu Noda, "Recent Progresses and Future Prospects of Two- and Three-Dimensional Photonic Crystals," 2006, *Journal of lightwave technology*, vol. 24, no. 12.