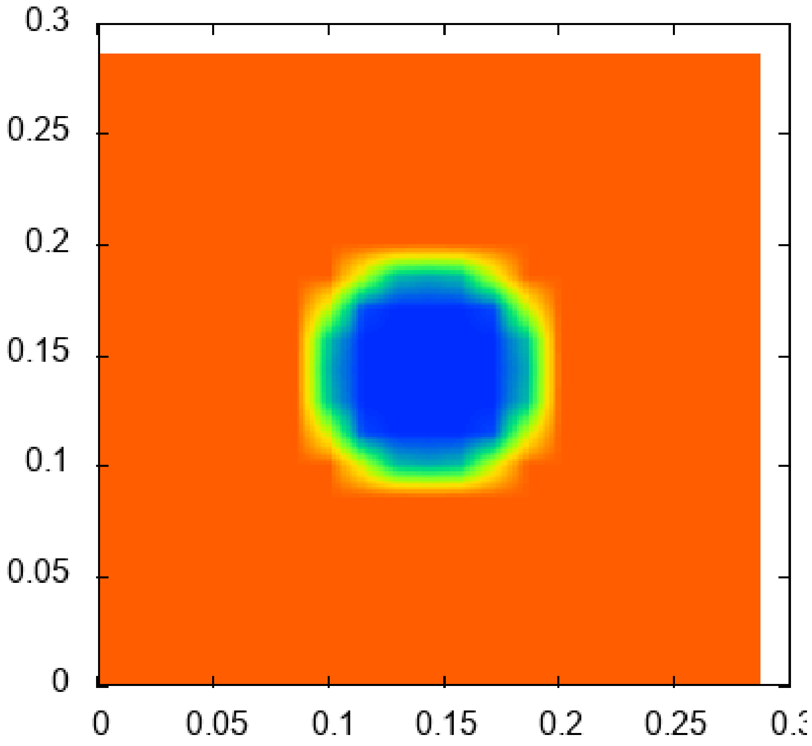
# Demonstration of PCSEL Kappa Calculation

# PCSEL Unit Cell

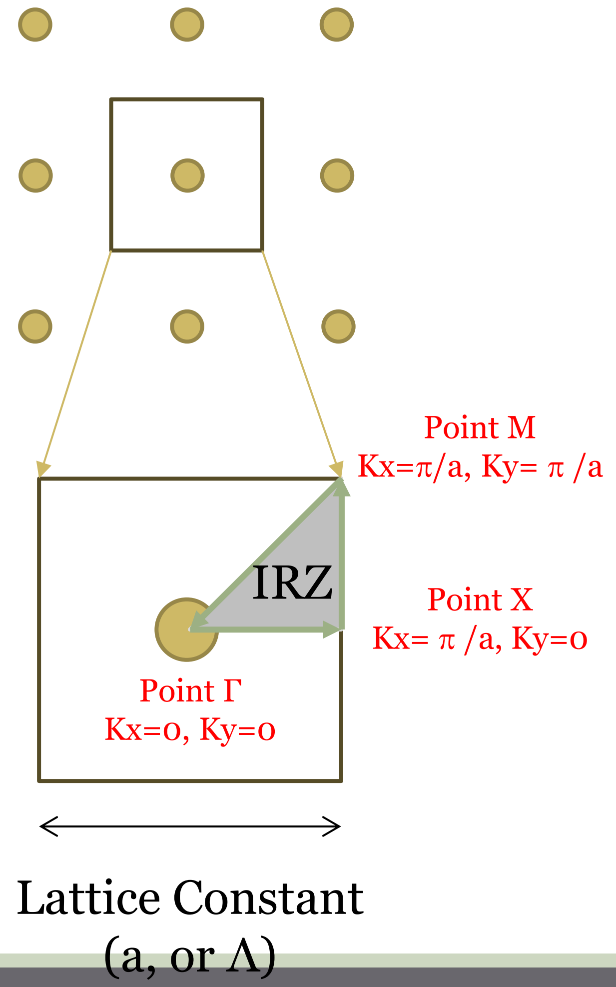
- Calculate the band diagram (dispersion relation) using a single PCSEL unit cell and periodic boundary conditions.




Single PCSEL cell

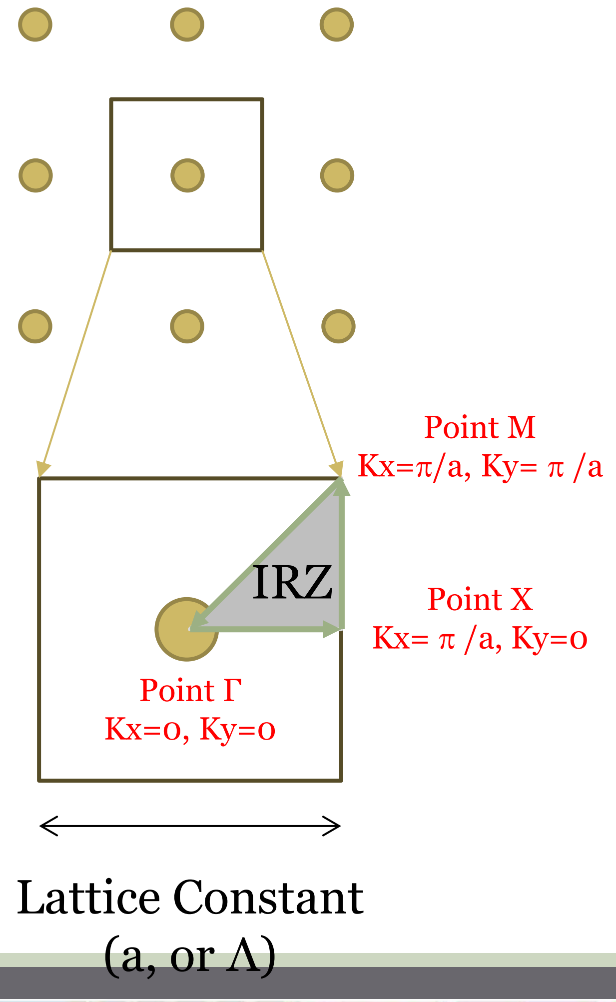
# PCSEL Cell

- Calculate the band diagram
  - Define the rectangular lattice
    - A Photonic Crystal (PC) in a rectangular lattice consists of
      - Dielectric arbitrary shape (in this case, a rod) placed in a periodic pattern in 2D
    - The unit cell
      - The smallest repeated section
      - To fully simulate the structure and calculate the band diagram, it is required to solve the eigenvalue problem over the outer perimeter of the Irreducible Brillouin Zones (IRZ)



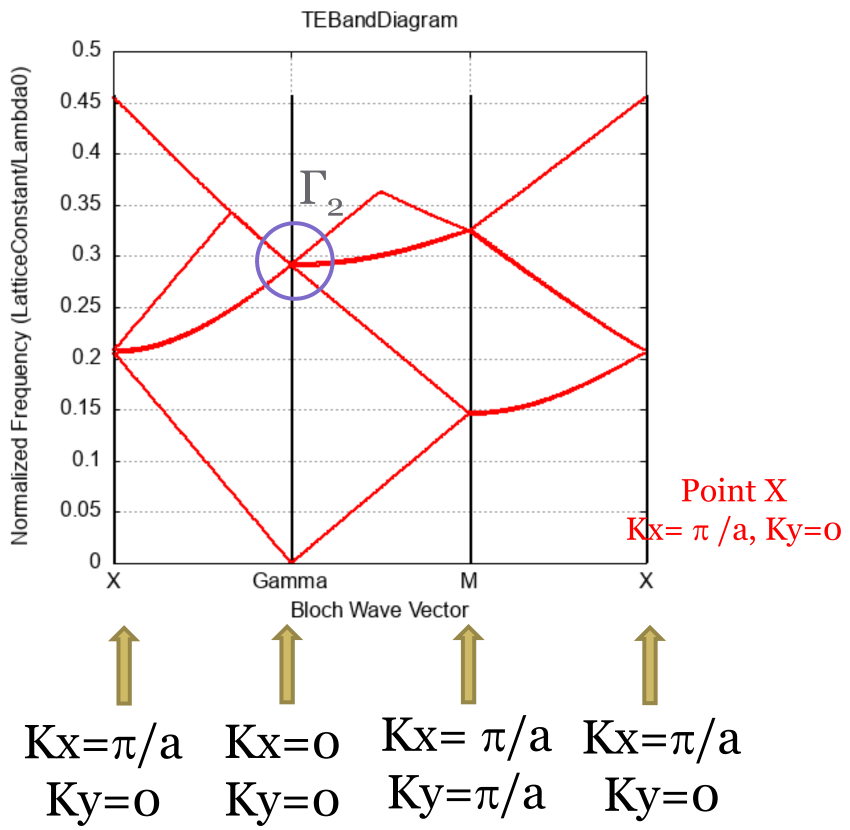
# PCSEL Cell

- Calculate the band diagram
  - Define the rectangular lattice
    - Define the Irreducible Brillouin Zones (IBZ)
      - Define the main points over the IBZ
        - Point Γ
        - Point X
        - Point M



# PCSEL Cell

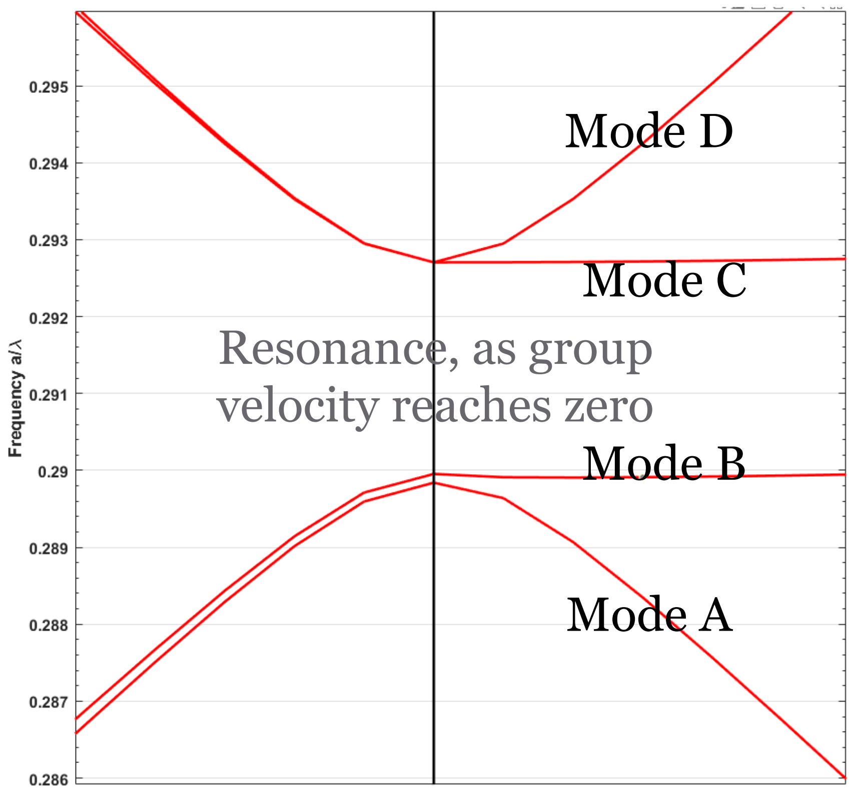
- Calculate the band diagram
  - Solve over the perimeter of the IBZ triangle
  - Define $\Gamma_2$ point



# PCSEL Cell

## Calculate band diagram

- Zooming near $\Gamma_2$
  - The dispersion curve is almost flat at $\Gamma_2$
  - 4 possible modes here
    - Mode A
    - Mode B
    - Mode C
    - Mode D
  - In this case, Modes C and D are degenerate at $\Gamma_2$ point

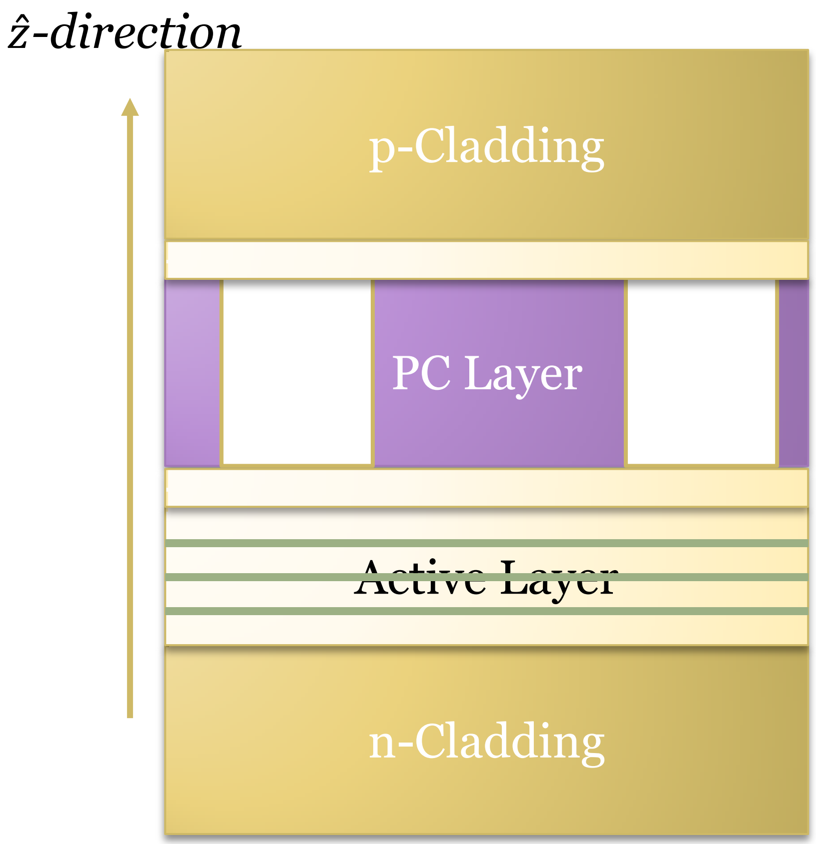



As the band diagram show, this point has a band gap between the optical modes

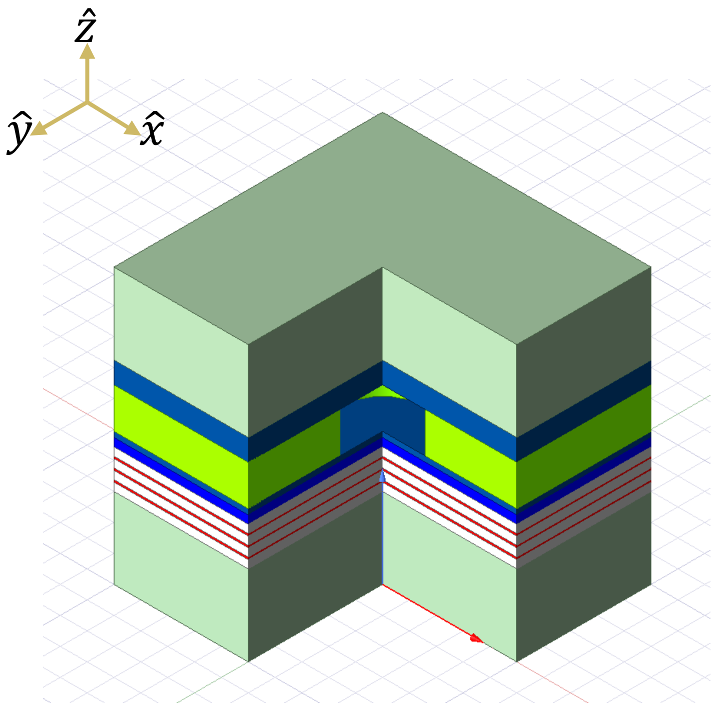
# PCSEL Cell Structure

## Input

- Starting point: 1D Layer file to define basic epitaxy
- Export epi sequence to 3D process simulator (CSUPREM)
- Use CSUPREM to generate the final hole pattern as part of the epitaxy steps



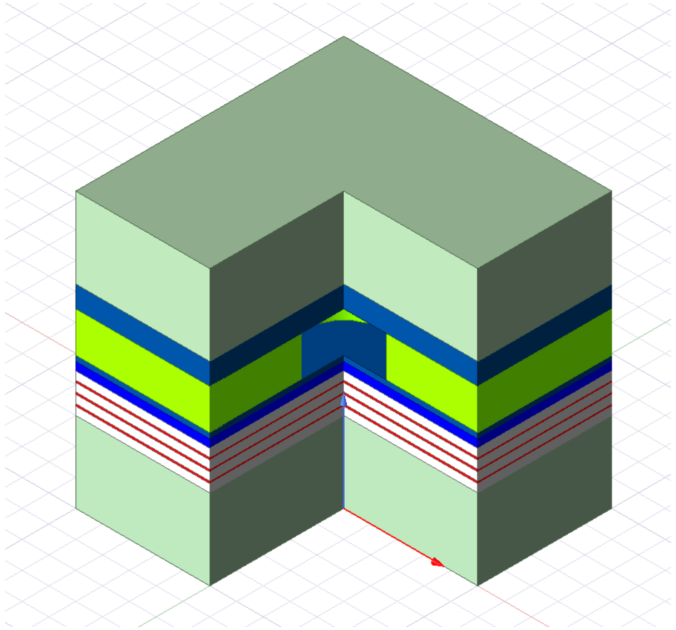

PCSEL Cell Cross-section




PCSEL cell Full 3D

# PCSEL Cell Structure

## Dimensions and Geometry

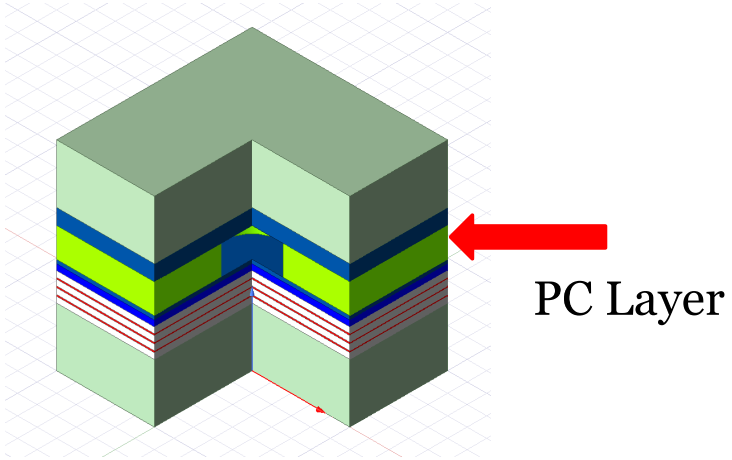


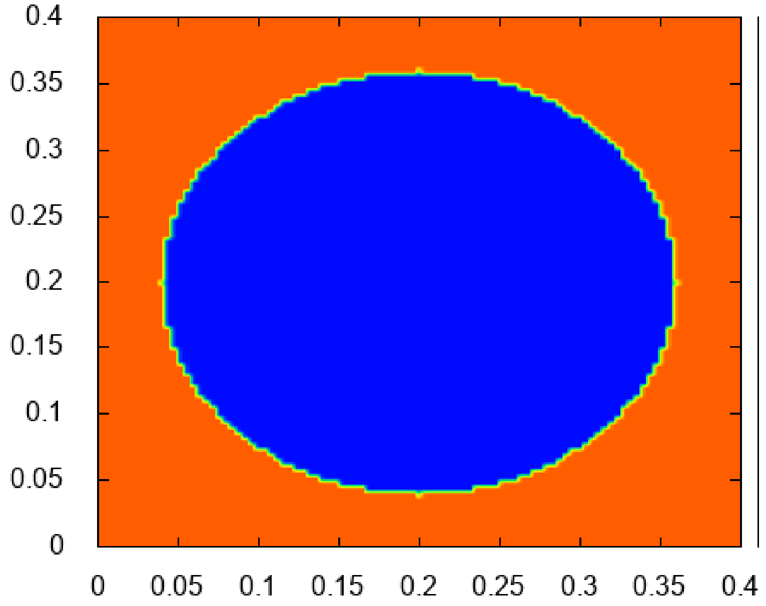
| | Material | Thickness |
|---|---|---|
| n-Cladding | $Al_{0.4}Ga_{0.6}As$ | 3.0 |
| MQW | GaAs | 0.030 |
| | $In_{0.2}Ga_{0.8}As$ | 0.008 |
| | GaAs | 0.030 |
| | $In_{0.2}Ga_{0.8}As$ | 0.008 |
| | GaAs | 0.030 |
| | $In_{0.2}Ga_{0.8}As$ | 0.008 |
| | GaAs | 0.030 |
| Separation layer (etch stop) | InGaP | 0.030 |
| | GaAs | 0.020 |
| PC Layer | InGap/Air | 0.150 |
| | GaAs | 0.080 |
| p-cladding | $Al_{0.4}Ga_{0.6}As$ | 3.0 |

# PCSEL Cell Structure

## Dimensions and Geometry

- Cross-section inside the PC layer
  - Pitch size (Λ): 0.40um
  - Defect radius: 0.16um (0.4 Λ)
  - Note: PC can take an arbitrary shape; in this case, we selected a circular PC-shape




Cross-section inside the PC layer

# PCSEL Cell Simulation

## Analysis

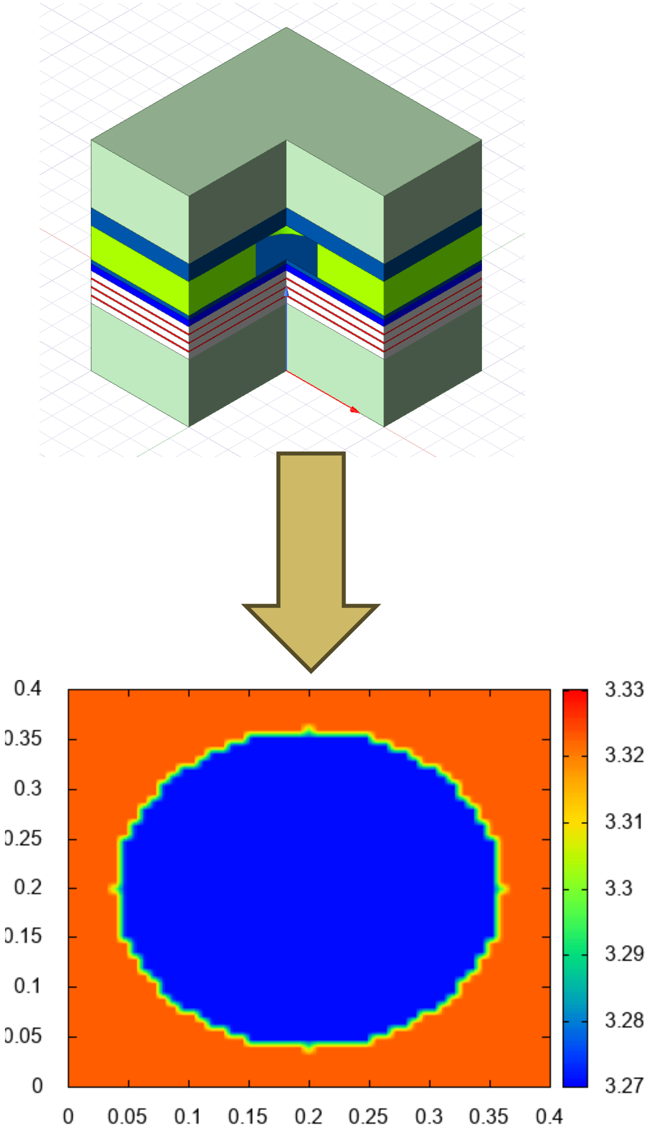
- Using PICS3D
  - Use "fdfd_pcsel" keyword to activate the coupling coefficient calculation.

```
$------- Part 2: Input statement -----------------------
$------- load mesh from csuprem output .aps file --------
include file=zmesh.zst &&
ignore1=load_mesh ignore2=output ignore3=export_3dgeo
load_mesh mesh_inf=pcsel.aps  suprem_import=yes
init_wave backg_loss=0.0 init_wavel=0.95 &&
wavel_range=(0.90,1.10)
microcavity_model fdfd_pcsel=yes average_index_dir=z
$------- Part 2: Input statement -----------------------
```

# PCSEL Cell Simulation

## 2D Results:

- Band diagram
  - Grid Size
    - The Full 3D grid size was selected to be:
      - 50 Grid points in x-direction
      - 50 Grid points in y-direction
      - 200 Grid points in z-direction
    - Reduce the structure using the effective refractive index to a 2D-grid*
      - 50 Grid points in x-direction
      - 50 Grid points in y-direction

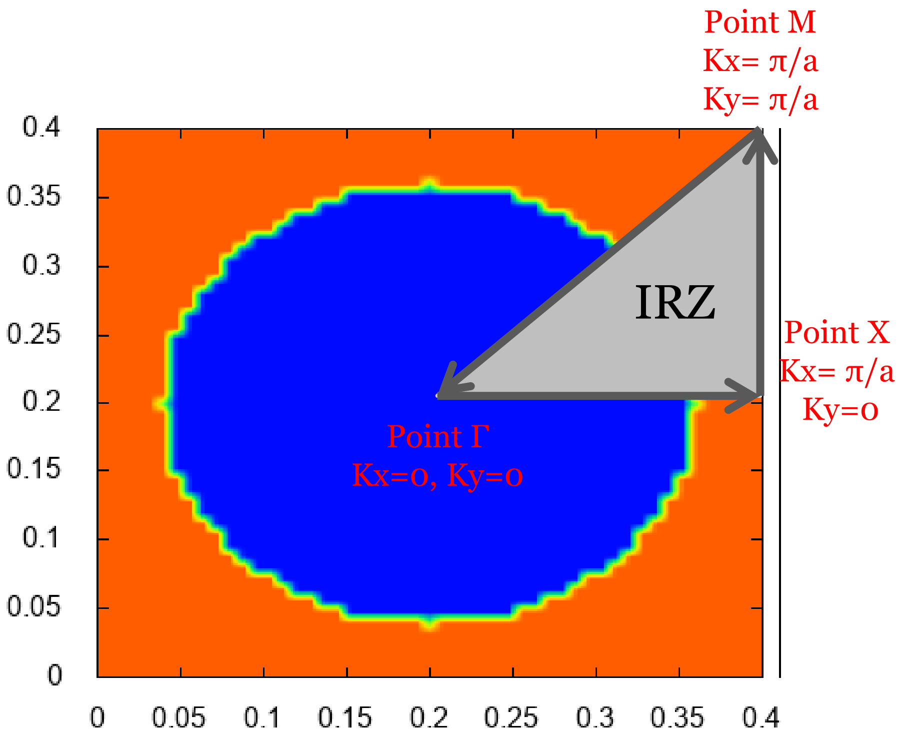



* DOI: https://doi.org/10.1103/PhysRevB.65.195306

# PCSEL Cell Simulation

## 2D Results:

- Band diagram
  - Applied Boundary condition
    - Periodic Boundary Condition (PBC)
  - Number of band-diagram points (around IRZ):
    - With different $k_x$,$k_y$ values, the eigenvalue problem will be solved around the perimeter of the IRZ to calculate the band diagram.

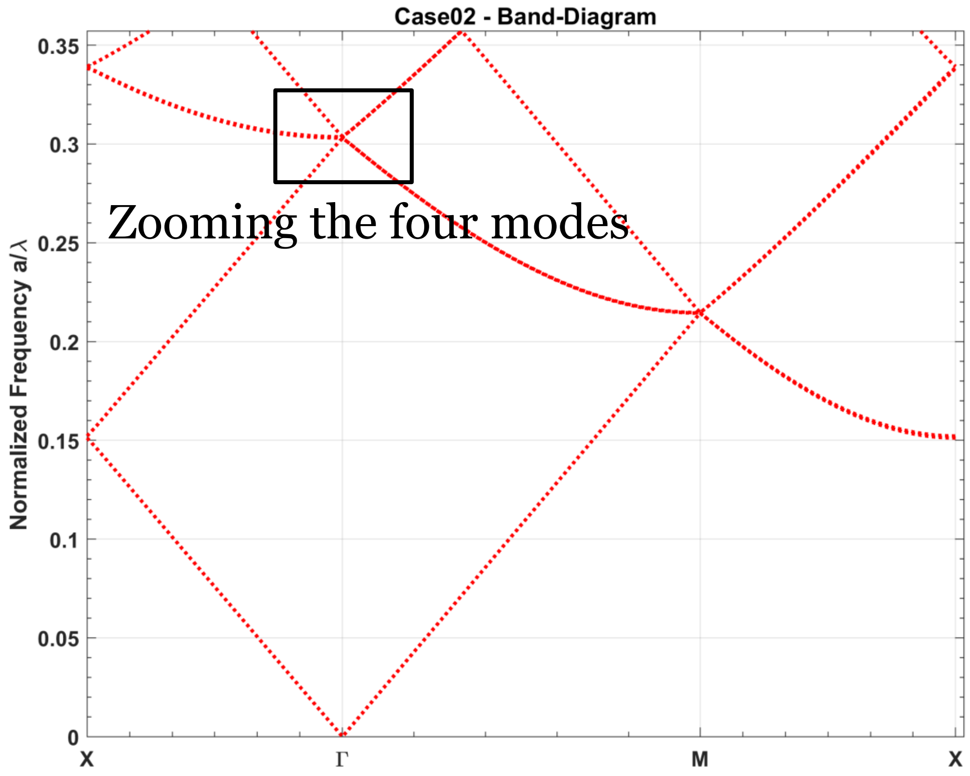



* DOI: https://doi.org/10.1103/PhysRevB.65.195306

# PCSEL Cell Simulation

## 2D Results:

- Band diagram
  - Number of band-diagram points (around IRZ):
    - Calculation starts from X-Point ($k_x=\pi/a$, $k_y=0$) and move towards Γ-Point ($k_x=0$, $k_y=0$).
    - Then move from Γ-Point to M-Point ($k_x=\pi/a$, $k_y=\pi/a$)
    - Lastly, go from M-Point ($k_x=\pi/a$, $k_y=\pi/a$) back to the X-Point
  - Since Only PBC used, no lossy modes and the band-diagram is clear



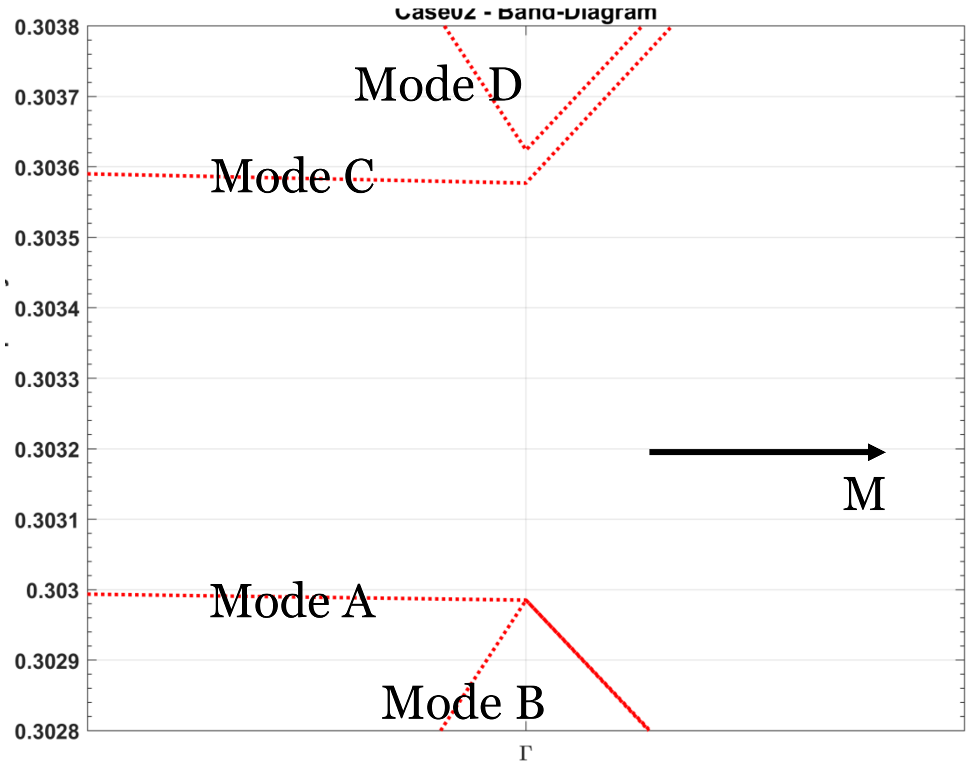

Full Band-Diagram

* DOI: https://doi.org/10.1103/PhysRevB.65.195306

# PCSEL Cell Simulation

## 2D Results:

- Band diagram
  - Γ-point results
    - A: 0.302834
    - B: 0.302834
    - C: 0.303421
    - D: 0.303468

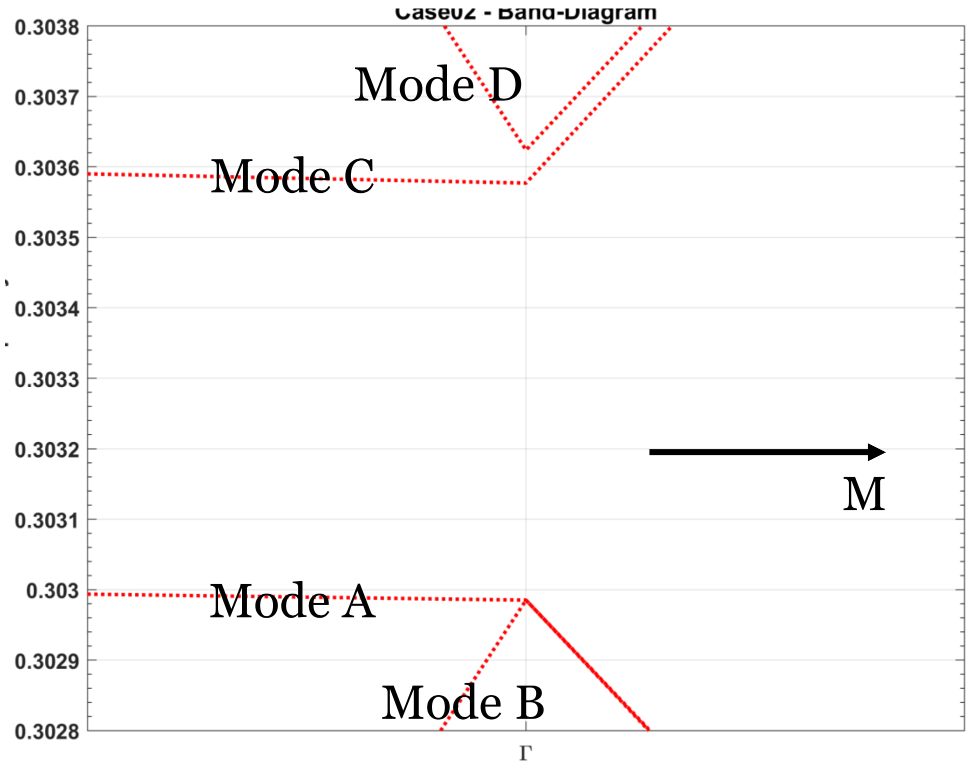



Zoom Band-Diagram around Γ

# PCSEL Cell Simulation

## 2D Results:

- Band diagram
  - Total Simulation Time: 13 seconds
    - Since the structure is reduced to a 2D structure, the analysis is fast.




Zoom Band-Diagram around Γ

# PCSEL Cell Simulation

## 2D Results:

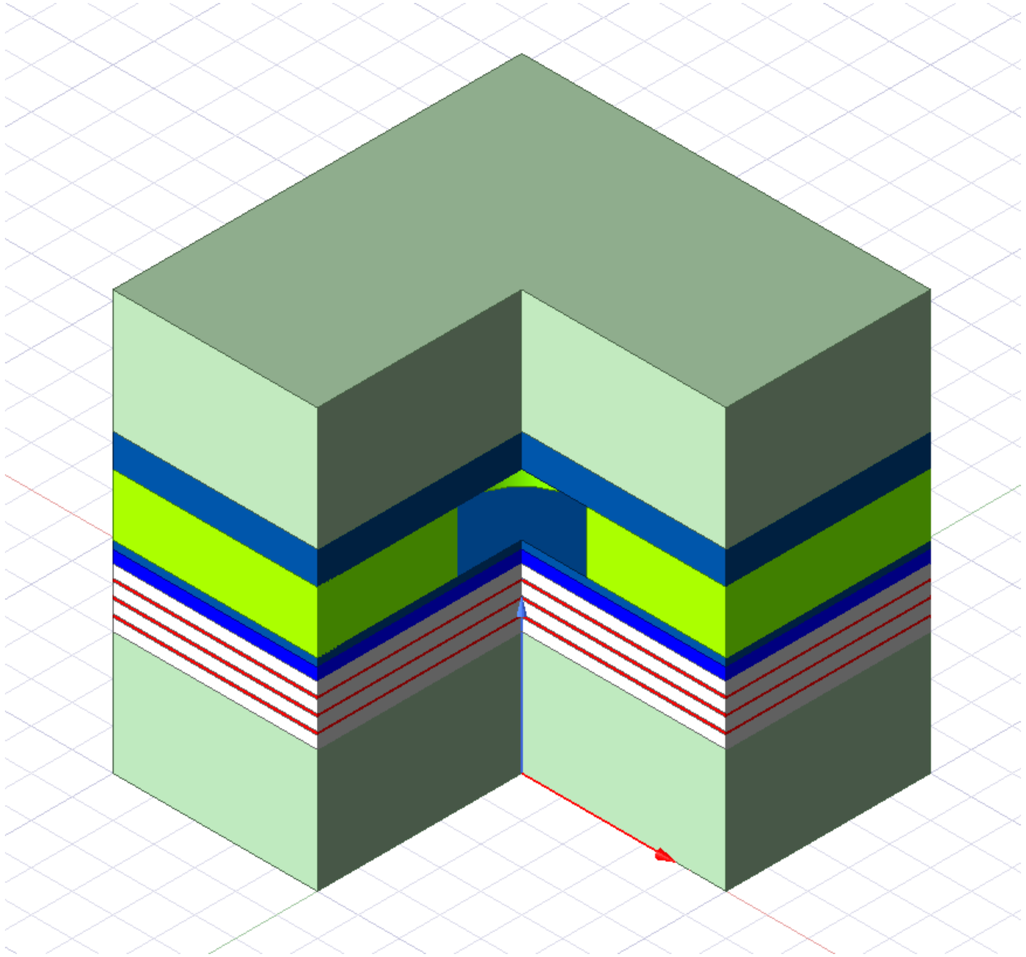
- Coupling Coefficients
  - Using the Γ-point in the band-diagram, the coupling coefficient can be calculated
    - Out-of-plane Coupling Coefficient (K1)
    - In-plane Coupling Coefficient (K3)

| | |
|---|---|
| In-Plane Coupling Coeff. | $1.583\times10^{+2}$ $cm^{-1}$. |
| Orthogonal Coupling Coeff. | $6.88\times10^{+2}$ $cm^{-1}$. |

# PCSEL Cell Simulation

## Results:

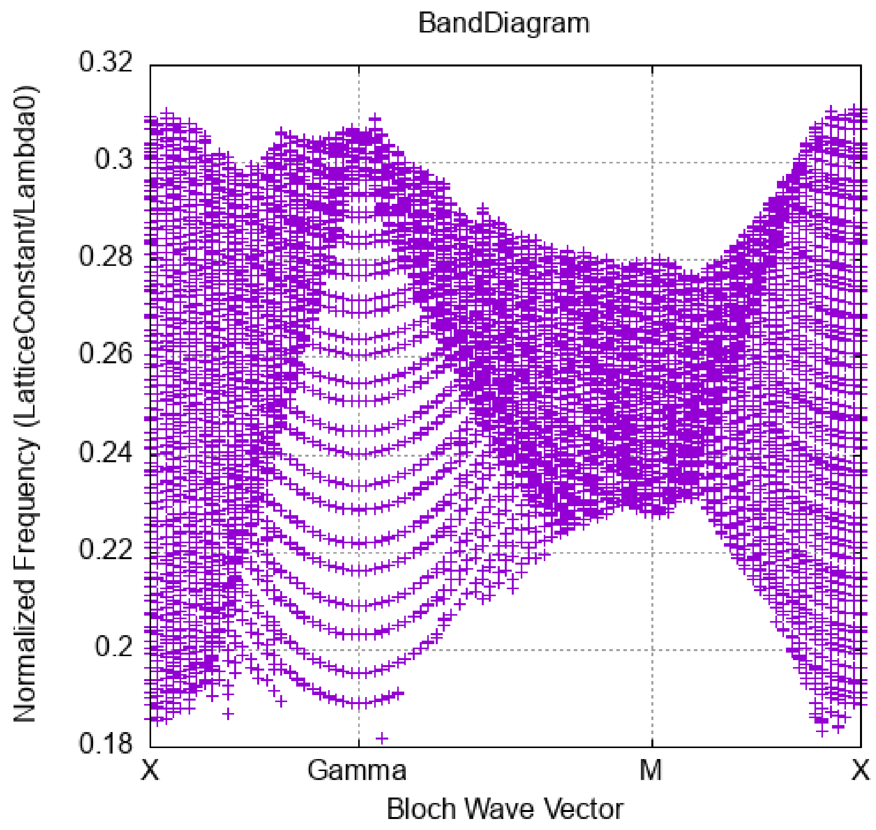
- Band diagram
  - Case02-Full 3D Analysis
    - Grid Size
      - To reduce memory usage, the full 3D grid size was selected to be:
        - 25 Grid points in x-direction
        - 25 Grid points in y-direction
        - 200 Grid points in z-direction
    - Boundary condition
      - X and Y-direction: PBC
      - Z-direction: Terminated with PML
      - Due to the PML, it is expected to have lossy modes and polluted band-diagram



# PCSEL Cell Simulation

## 3D Results:

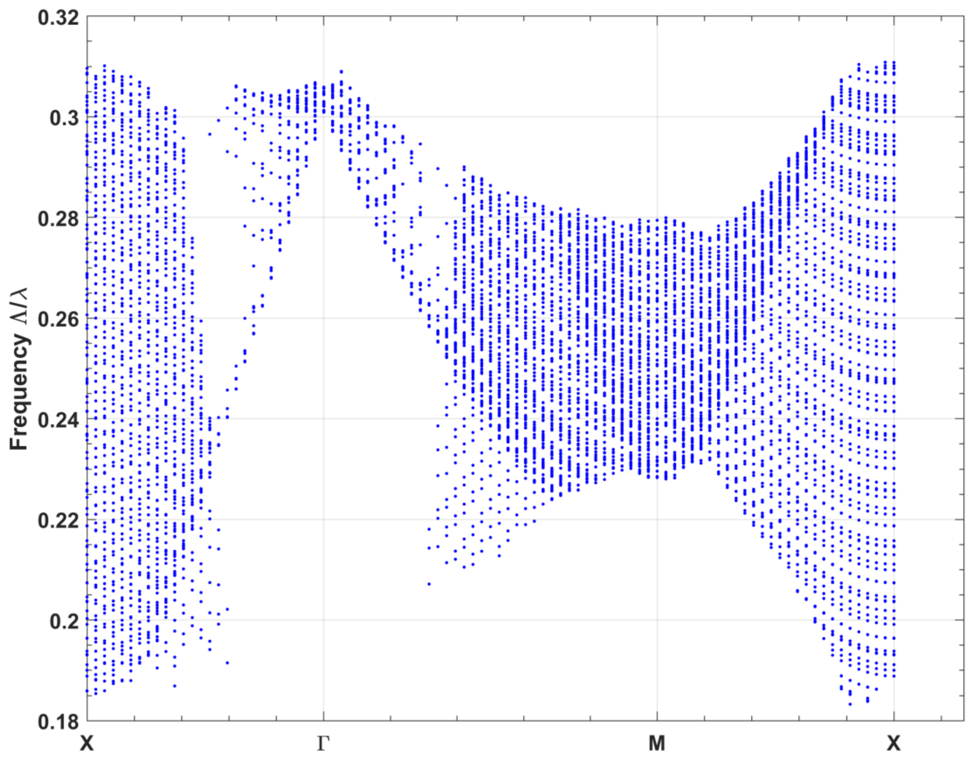
- Band diagram
  - Number of band-diagram points (around IRZ):
    - The eigenvalue problem will be solved more than 90 times.
    - Each run will solve the full 3D structure
    - Due to the 3D structure, the band diagram looks more complicated



# PCSEL Cell Simulation

## 3D Results:

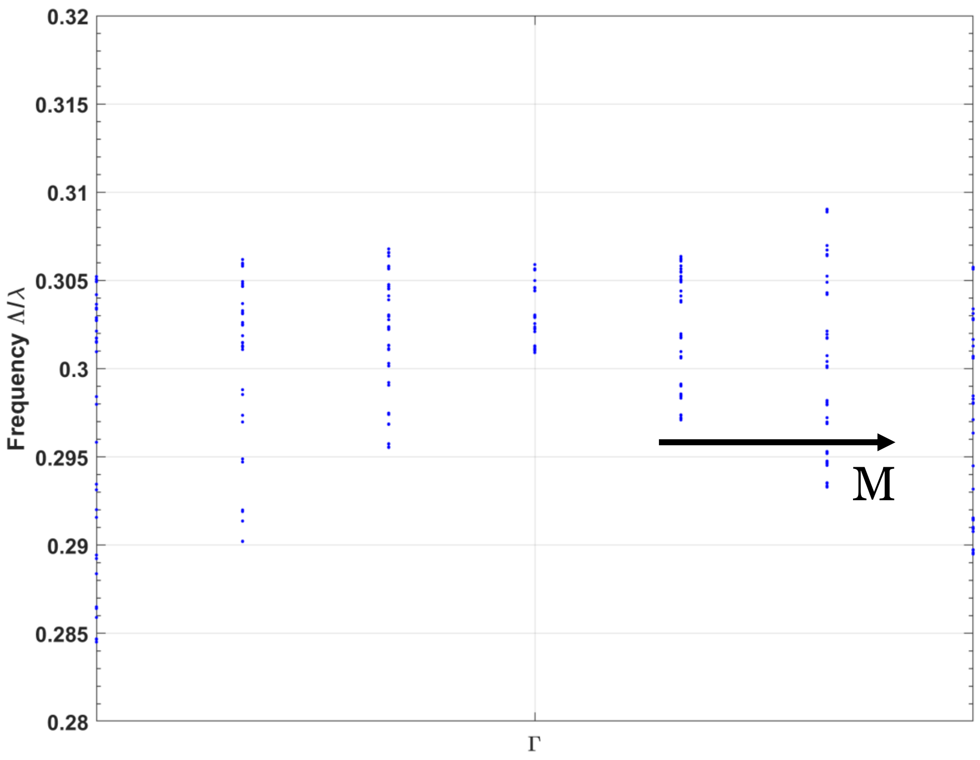
- Band diagram
  - Number of band-diagram points (around IRZ):
    - The eigenvalue problem will be solved more than 90 times.
    - Each run will solve the full 3D structure
    - Due to the 3D structure, the band diagram looks more complicated
      - After removing lossy modes



# PCSEL Cell Simulation

## 3D Results:

- Band diagram
  - Total Simulation Time: more than 24 hours
  - Simulation time varies depending on the complexity of the unit cell and the mesh.
  - Increasing the mesh size increases both the memory and simulation time




Zoom Band-Diagram around Γ

# PCSEL Cell Simulation

## 3D Results:

- Coupling Coefficients
  - Using the Γ-point in the band-diagram, the coupling coefficient can be calculated
    - Out-of-plane Coupling Coefficient (K1)
    - In-plane Coupling Coefficient (K3)

| | |
|---|---|
| In-Plane Coupling Coeff. | $1.522 \times 10^{+2}$ $cm^{-1}$. |
| Orthogonal Coupling Coeff. | $6.50 \times 10^{+2}$ $cm^{-1}$. |

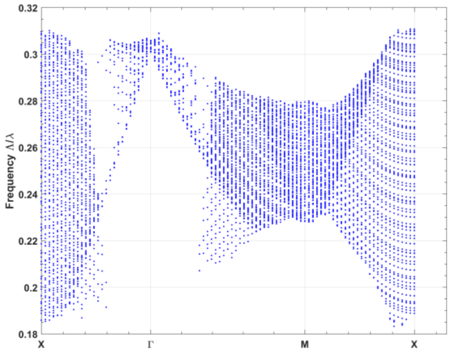
# PCSELL Cell Simulation

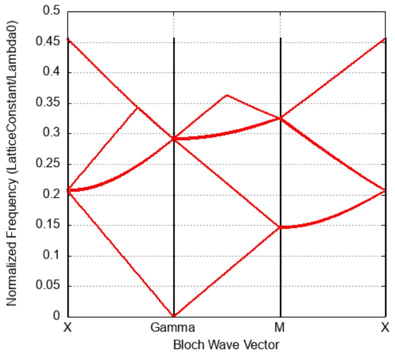
## Full 3D unit cell simulation

- Grid Size: 25x25x200
- BC: PBC/PBC/PML
- Simulation time: >24hours!

## 2.5D cell simulation

- Grid Size 50x50
- BC: PBC/PBC Simulation time: around 10 secs




| | 2D Analysis | 3D Analysis |
|---|---|---|
| In-Plane Coupling Coeff. | $1.583\times10^{+2}$ $cm^{-1}$. | $1.522\times10^{+2}$ $cm^{-1}$. |
| Orthogonal Coupling Coeff. | $6.88\times10^{+2}$ $cm^{-1}$. | $6.50\times10^{+2}$ $cm^{-1}$. |

Both simulation presents close results around the Γ points

# Thank you